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REACTIVITY/VOLATILITY CLASSIFICATION
OF
SELECTED ORGANIC CHEMICALS:
EXISTING DATA

by

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This study deals with the reactivity/volatility classification of some 118 organic chemicals specified by the U. S. Environmental Protection Agency (EPA). The classification system has been developed based on existing and available information. It was clear at the outset that little or no experimental data were available for a significant fraction of these chemicals. In such cases we relied heavily on our ability to make valid predictions, based on sound physico-chemical principles. As requested by EPA, a three-tiered individual, as well as composite, classification scheme of the reactivity and volatility of these 118 chemicals was developed. The three-tiered classification system was conceived as follows: Class I (26 chemicals): These chemicals are sufficiently nonvolatile or unreactive so that they may not participate in photochemical smog formation; Class II (17 chemicals): Chemicals that are borderline cases, or for which available data are inadequate to draw definitive conclusions; Class III (75 chemicals): These chemicals are both reactive and volatile, and can participate in processes of smog formation.

Because of extensive shortcomings in existing information a number of recommendations were made to bridge current information gaps.

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ABSTRACT

This study deals with the reactivity/volatility classification of some 118 organic chemicals (including isomers and one solvent mixture) specified by the U.S. Environmental Protection Agency (EPA). The classification system has been developed based on existing and available information. It was clear at the outset that little or no experimental data were available for a significant fraction of these chemicals. In such cases we relied heavily on our ability to make valid predictions, based on sound physico-chemical principles. As requested by EPA, a three-tiered individual, as well as composite, classification scheme of the reactivity and volatility of these 118 chemicals was developed. It is recognized that the degree of photochemical involvement of chemicals cannot be rigorously compartmentalized into discrete classes; nevertheless, a practical classification system is considered useful from a control strategy viewpoint. The three-tiered classification system was conceived as follows:

Class I (26 chemicals): These chemicals are sufficiently nonvolatile or unreactive so that they may not participate in photochemical smog formation.

Class II (17 chemicals): Chemicals that are borderline cases, or for which available data are inadequate to draw definitive conclusions.

Class III (75 chemicals): These chemicals are both reactive and volatile, and can participate in processes of smog formation.

It is found that smog chamber data for low reactivity organic chemicals may not be directly applicable to ambient conditions. Because of extensive shortcomings in existing information a number of recommendations were made to bridge current information gaps.

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SECTION 1

INTRODUCTION

Current strategies to control photochemical air pollution rely on abating the emission of volatile organic compounds (VOCs). Because VOCs differ significantly in their ability to produce oxidants, a strategy based on the control of those compounds which manifest themselves most strongly in smog formation, rather than indiscriminate control, clearly constitutes a superior technical approach.

Three major factors determine the ozone- or oxidant-forming ability of an organic chemical:

- Ambient concentrations (or emissions)
- The ability of the organic chemical and its intermediate products to remain in the gas phase (volatility)
- The ability of the organic chemical to oxidize in the atmosphere (typically, by reacting with OH or O_3) and the efficiency of the oxidation products to form ozone (reactivity).

This study deals with the reactivity/volatility classification of some 118 organic chemicals (including isomers and mixtures) specified by the Environmental Protection Agency (EPA). These compounds include the 101 compounds produced in largest volume in the U.S. as well as several additional compounds used by the paint and coatings industry. The classification system has been developed based on existing and available information. It was clear at the outset that little or no experimental data were available for a significant fraction of these chemicals. In such cases we relied heavily on our ability to make valid predictions, based on sound physico-chemical principles. As requested by EPA, a three-tiered individual, as well as a composite, classification scheme of the reactivity and volatility of these chemicals was developed. It is recognized that photochemical involvement of organic chemicals cannot be rigorously compartmentalized into discrete classes. Nevertheless, such a classification system is a useful, practical tool from a control strategy viewpoint. For those cases where existing information does not allow any definitive conclusions, a research protocol that bridges many of the shortcomings of the current information needs to be developed. It is noted that the regulatory objective is to classify chemicals as those that either "contribute to smog" or those that "do not contribute to smog." The middle category is created as a practical necessity when the above assignments are not possible for lack of reliable information.

SECTION 2

OBJECTIVES

The overall objectives of this study are the following:

- Develop a three-class reactivity scale for a list of 118 specified organic chemicals
- Develop a three-class volatility scale for a list of 118 specified organic chemicals
- Develop an integrated three-class scale that takes into account both reactivity and volatility considerations

These three-tiered scales are constituted as follows:

- Class I: Compounds that are unreactive or nonvolatile and do not contribute to smog formation.
- Class II: Compounds that are borderline cases or for which insufficient information is available to draw definitive conclusions.
- Class III: Compounds that are reactive and volatile, and contribute to smog formation.

SECTION 3

GENERAL TECHNICAL APPROACH

REACTIVITY CLASSIFICATION

Hydrocarbon reactivity has been defined in many objective and subjective ways. The most commonly used objective criteria are maximum ozone formation, rate of hydrocarbon depletion, NO (or NO_2) oxidation rates, and analysis, and concentrations of photochemical products. The most common subjective criterion employs eye irritation as an index of oxidants in a simulated smog system. It is now well recognized that photochemical air pollution is not limited to effects of ozone alone, but rather to a broad category of secondary products (EPA, 1978; Altshuller, 1982). However, ozone is a useful surrogate for the effects of photochemical pollution, and a specific national air quality standard (0.12 ppm O_3 - hourly standard not to be exceeded more than once in a year) currently exists. Keeping this in mind, we have given most attention to the following objective parameters --

- Maximum O_3 yield
- Organic chemical (OC) depletion rate
- NO (or NO_2) oxidation rate
- Product analysis

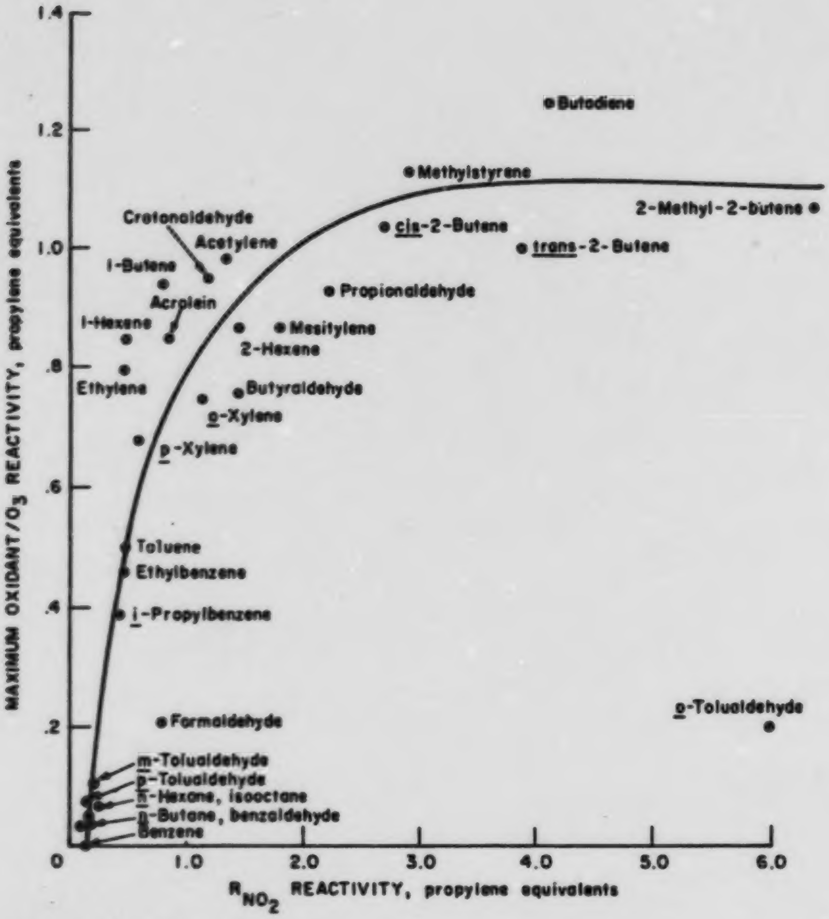
It is recognized that the above objective parameters are not absolute but are dependent on factors such as OC concentration, OC/NO_x (ppmv/ppmv unless otherwise specified) ratio, light intensity and temperature.

The above parameters were often directly available from smog chamber studies. A wide range of OC and NO_x initial concentrations had been employed in these studies. Typical initial OC/NO_x (ppmv/ppmv) ratios varied from 2 to 20, but ratios of <1 and >100 were also encountered. Chemicals that could be shown to produce O_3 concentrations in excess of 0.12 ppm with an initial OC concentration of ≤ 4 ppm and any OC/NO_x ratio have been called reactive (Class III). OC depletion rates and NO oxidation rates were also typically reported in most smog chamber studies. There were very few instances where the OC depletion rates and NO oxidation rate contradicted the results of ozone formation. In most, but not all, cases the reasons for these discrepancies could be explained.

Figure 1 shows the relationship between reactivity based on maximum ozone formation and the rate of NO_2 formation (Dimitriades et al., 1975). Similarly, Figure 2 shows the correlation of maximum OC disappearance rate and the maximum rate of NO_2 disappearance (Laity et al., 1973). Although linear relationships are not implied, it is apparent that high organic chemical reactivity, high NO oxidation rate, and high O_3 formation are all manifestations of the processes that lead to smog formation.

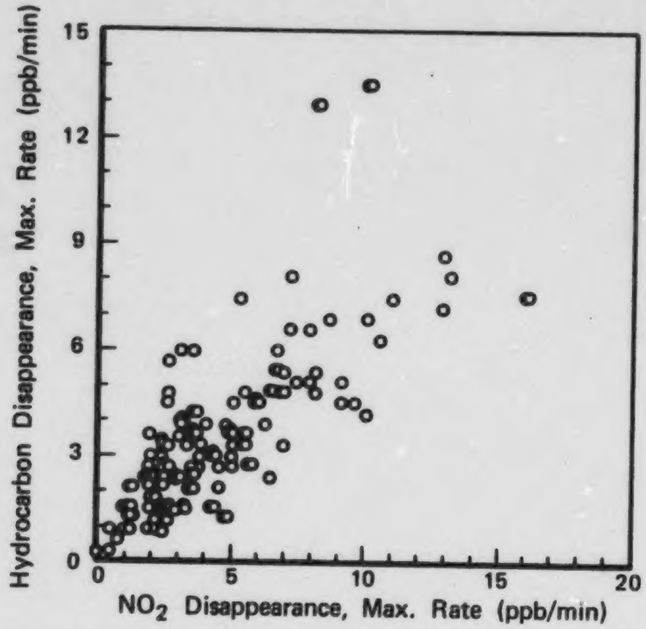
Figures 3 and 4 further show the significance of the initial OC/NO_x ratio in ozone formation. The figures are derived from data presented by Altshuller and Bufalini (1971) and Sickles et al. (1980). It is obvious that a chemical can be erroneously considered nonreactive when a wide range of OC/NO_x ratios are not considered. Since a great deal of smog chamber data has been obtained under conditions of low initial OC/NO_x ratios (2 to 10) and relatively short irradiation times (3 to 7 hours), this aspect was especially kept in mind in assigning reactivities. When irradiations at high OC/NO_x ratios (>20) had also been performed, such data were decisive even when low OC/NO_x data showed little or no reactivity.

Over the years, it has also become apparent that OC depletion is most dependent on reaction with the hydroxyl radical (OH) (Altshuller and Bufalini, 1971; Niki et al., 1973; Darnall et al., 1976). Figure 5 shows this relationship for a number of compounds whose disappearance rates have been measured in smog chambers (Pitts et al., 1978). It is acknowledged that alkenes may react with O_3 and aldehydes may photolyze at significant rates. Nevertheless, reactivity analysis is possible based on reaction with OH radicals in the absence of smog chamber data. Although exceptions exist, irradiations with NO_x of a mixture of n-pentane, m-xylene and trans-2-butene (Winer et al., 1979) seem to



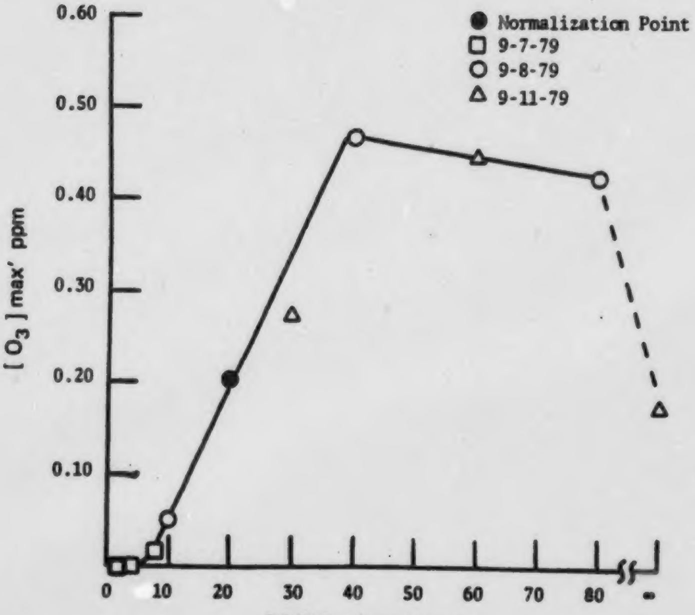
SOURCE: DIMITRIADES, et al. (1975)

Figure 1. Correlation of maximum oxidant/O_3 and R_{NO_2} reactivities



SOURCE: LAITY, et al. (1973)

Figure 2. A sample correlation plot of NO_2 and hydrocarbon disappearance rates



SOURCE: SICKLES, et al. (1980)

Figure 3. Maximum ozone concentrations produced by the propane-NO_x-air irradiations in an outdoor smog chamber at various OC to NO_x ratios

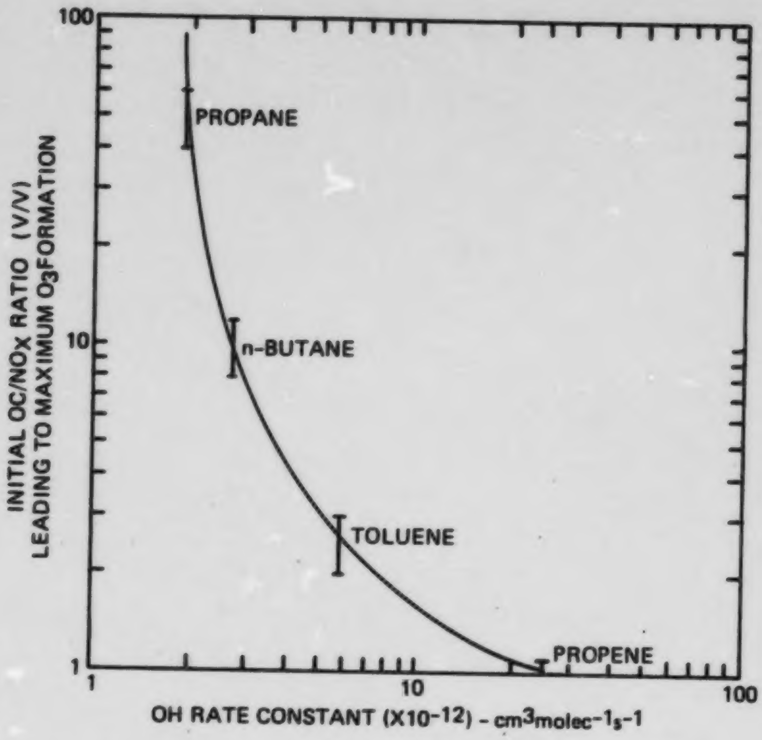
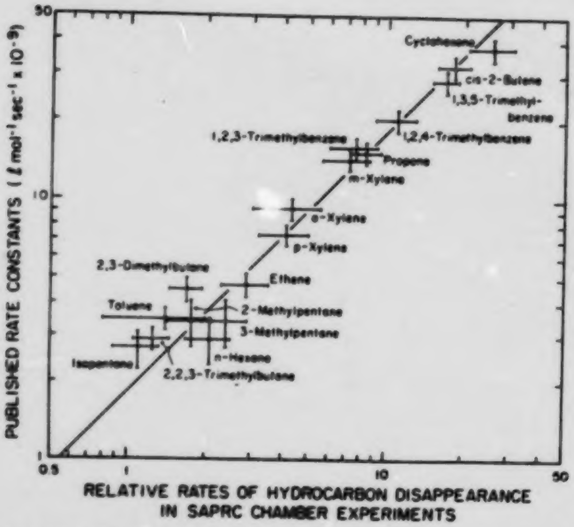
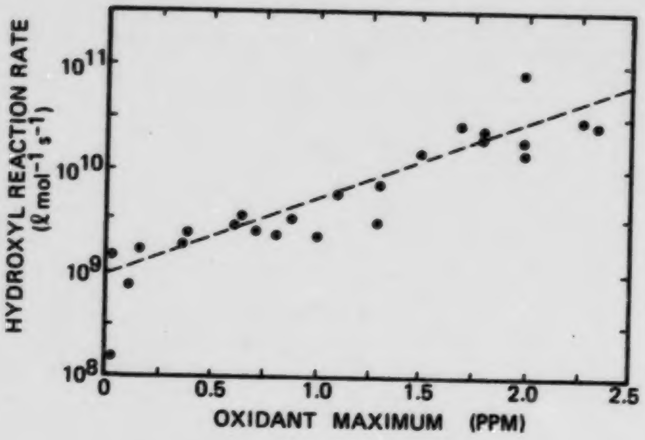


Figure 4. Relationship between OH rate constant and initial organic chemical to NO_x ratio needed for maximum O_3 formation



SOURCE: PITTS, et al. (1978)

Figure 5. Comparison of relative hydrocarbon disappearance rates (n-butane=1) and hydroxyl radical rate constant



SOURCE: ADAPTED FROM FARLEY, (1978)

Figure 6. Hydrocarbon reactivity vs. oxidant maximum

suggest that O_3 and PAN yields depend primarily on the OH radical reactivity. This observation is further confirmed by Akimoto and Sakamaki (1983) for the case of propylene-NO_x system. Figure 6 shows results compiled by Farley (1978) that further support this contention.

In summary, we have depended heavily on smog chamber irradiations for our reactivity classifications. These data have been complemented with OH reactivity to better understand those cases that are exceptions to general rules. Instances where no smog chamber data were available are identified. In such cases, we have used OH reactivity as the primary guiding criterion, although reactions with O_3, O, NO_3 as well as photolysis are considered when appropriate. Exceptions are dealt with on a case-by-case basis. These few exceptions deal specifically with free radical scavengers, such as phenol, aniline, naphthalene (Gitchell, 1974; 1974a), as well as instances where smog chamber systems may not simulate ambient conditions (e.g., perchloroethylene).

Although there are exceptions, our findings on reactivity can be broadly stated as follows:

Class I: Organics where direct (smog chamber) data shows O_3 formation significantly less than 0.12 ppm, and the chemical has a measured or calculated depletion rate that is less than ethane.

Class II: Direct evidence shows O_3 formation near 0.12 ppm or depletion rates are 1 to 5 times that of ethane.

Class III: Chemicals where direct evidence of O_3 formation in excess of 0.12 ppm (initial conditions of OC <4 ppm and any OC/NO_x ratio) is available, and/or measured or calculated depletion rates are larger than 5 times that of ethane, or chemicals for which no direct or indirect evidence on reactivity exists.

The reasons that led to these divisions, and the specific exceptions, will become clear during the Discussion of Results in Section 5. We note here that for ethane and for species 2 to 5 times as reactive as ethane, limited experimental evidence was available, but the results were not unequivocal. Only for chemicals more than 5 times as reactive as ethane did convincing evidence of reactivity emerge from available data. We also point out that for low reactivity chemicals, the reaction rate constants are often uncertain to within a factor of 2.

VOLATILITY CLASSIFICATION

The photochemical reactivity of ozone precursors in the atmosphere depends in part on the gas-phase distribution of reactive species. Vapor phase organics may be removed from the atmosphere under ambient conditions by water droplets or suspended particulate matter (aerosols). The effectiveness of these sinks will determine the amount of chemical available for gas-phase reactions.

Chemical species dissolved in dilute solutions partition between the vapor phase and the condensed phase depending on their relative vapor pressure and solubility. The ambient phase distribution can be quantified by Henry's law

$$P=HC$$

where P is the partial pressure of the chemical in air, C is the solute concentration of the chemical dissolved in solvent, and H is Henry's constant. Henry's constant is then a temperature-dependent measure of the phase distribution for a chemical at the temperature of the partial pressure and solubility given. In the absence of measured values of H, the Henry's constant can be calculated from the saturated vapor pressure and solubility.

Phase distribution depends on the mass transfer rates of a substance across the liquid- and gas-phase boundary layers. Liss and Slater (1974) have suggested typical mass transfer coefficient values for O_2 and H_2O transfer. Based on these parameters, a chemical with high vapor pressure and/or low solubility ($H > 5 \times 10^{3}$ atm m^{3} mol^{-1}) is 95% controlled by liquid phase resistance, while low vapor pressure and/or high solubility ($H < 1 \times 10^{-5}$ atm m^{3} mol^{-1}) results in 95% resistance by the gas phase. Chemicals have been classified as high, intermediate, or low volatility compounds on the basis of their Henry's constants (Smith et al., 1980, 1981). This approach is not directly applicable to the partitioning of a chemical into solution that is already in the gas phase because the gas/liquid equilibrium time is far greater than reaction or removal rates in the atmosphere.

Experimental determinations in polluted atmospheres have been made by Cautreels and Van Cauwenberghe (1976, 1978) and Broddin et al. (1980) of the distribution of organic pollutants between airborne particulate matter and the gas phase. Eichmann et al. (1979, 1980) also conducted similar measurements for naturally occurring n-alkanes in unpolluted marine air. The Van Cauwenberghe and Broddin studies found that lower molecular weight compounds with high vapor pressures were predominantly present in the gas phase, although the maximum molecular weight and minimum vapor pressure varied among chemical classes. The vapor pressure limit, above which a class of chemicals partitioned into the gas phase, ranged over several orders of magnitude. Chemicals with vapor pressures above 10^{-6} atm consistently were found predominantly in the gas phase, and can therefore be classified as high volatility (Class III) compounds. Although the overall results of Eichmann et al. are in substantial disagreement with the Van Cauwenberghe and Broddin studies, there is agreement that species with vapor pressures of $\geq 10^{-6}$ atm will be found essentially in the gas phase. Some gaseous chemicals are highly soluble in water and others may be preferentially adsorbed by aerosols. The small amount of water content under typical smog conditions (relative humidity <70%) and relatively low particulate abundances in the ambient atmospheres (Heicklen, 1981) are unlikely to significantly remove the gaseous reservoir of such chemicals.

Heicklen (1981) has shown that the removal rate of atmospheric species is related to the turnover rate of atmospheric particulate matter. In the absence of reaction in water droplets or on aerosol surfaces, vapor pressures less than 4×10^{-9} atm are required for complete removal by particulate matter. Under typical environmental conditions, chemicals with vapor pressures less than about 10^{-8} atm should result in nearly complete (>75%) removal. These chemicals have been classified as low volatility (Class I) compounds, and exhibit partitioning predominantly into the condensed phase. This cutoff of $\leq 10^{-8}$ atm vapor pressure for nonvolatile species is in good agreement with the results of Broddin et al. (1980). Unfortunately, it is in disagreement with the results of Eichmann et al. (1979, 1980) who find even C_{28} alkanes (vapor pressure 7×10^{-11} atm) primarily in the gas phase. Their results are shown in Figure 7, and clearly suggest that more than 95% C_9-C_{28} alkanes exist in the vapor phase. Table 1 summarizes the results of Broddin et al. (1980) where all chemicals with vapor pressures equal to or greater than tetracosane (C_{24}, V.P.=1.3×10^{-8} atm) are found exclusively in the aerosol phase.

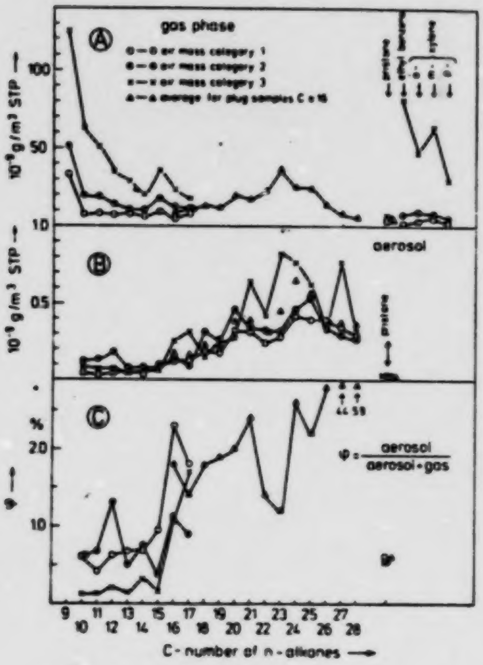
We have chosen the 10^{-8} atm vapor pressure as the cutoff for Class I (nonvolatiles) primarily because it conforms with the theoretical analysis of Heicklen (1981) as well as the experimental results of Broddin et al. (1980). Unlike the Eichmann et al. (1979, 1980) studies, the Broddin studies are performed in typical urban atmospheres. Here the aerosol composition and density may be such that high molecular weight species can be adsorbed onto available surfaces. Eichmann's studies were performed in remote marine atmospheres and are not directly applicable to polluted air. From these studies it is evident that volatility is highly dependent on the type of the aerosol mix available for condensation and adsorption.

Vapor pressures between 10^{-8} and 10^{-6} atm result in varying degrees of partitioning depending on chemical structure, functional groups, and atmospheric conditions. These have been classified as intermediate volatility (Class II) compounds. Class II has also been designated for organics of uncertain phase distribution, or insufficient information.

The volatility of each chemical has been classified as follows:

Class I: Organics with clearly greater percent occurrence in the condensed phase (>75% condensed phase) under ambient conditions (vapor pressure $<1 \times 10^{-8}$ atm).

Class II: Organics with intermediate phase distribution in ambient air (1×10^{-8} atm < vapor pressure < 1×10^{-6} atm), and organics for which volatility or phase distribution evidence does not exist.



SOURCE: EICHMANN, et al. (1979)

Figure 7. Distribution of C_9-C_{28} n-alkanes and other select chemicals in the aerosol and gas phase

Table 1. Distribution of aliphatic hydrocarbons between aerosol (A) and gas (G) phase at Ghent (residential), μg/1000 m^3

Compound	January		February		March		July		August		September	
	A	G	A	G	A	G	A	G	A	G	A	G
Hexadecane	2.38	40	1.51	36	0.21	94	—	306	—	251	0.81	154
Heptadecane	1.20	39	1.56	37	0.49	41	—	362	—	346	0.78	335
Octadecane	1.63	22	2.75	22	0.75	47	—	245	1.59	130	1.30	118
Nonadecane	1.26	3	1.00	3	0.30	1	1.87	38	1.05	13	0.75	16
Eicosane	2.91	—	1.90	1	0.33	4	1.20	7	0.96	10	0.63	2
Heneicosane	4.93	1	3.33	1	0.90	2	1.79	13	1.13	6	0.59	—
Docosane	9.95	—	8.69	—	1.96	1	2.10	1	1.53	3	1.44	9
Tricosane	13.73	—	10.33	—	2.67	—	5.31	1	3.17	4	3.99	1
Tetracosane	19.34	—	12.60	—	4.94	—	4.42	—	4.22	—	6.41	—
Pentacosane	18.51	—	9.44	—	4.07	—	7.95	—	8.63	—	7.63	—
Hexacosane	18.62	—	6.86	—	5.01	—	2.58	—	3.65	—	4.90	—
Heptacosane	18.64	—	5.18	—	4.78	—	6.14	—	5.35	—	5.81	—
Octacosane	17.26	—	4.80	—	2.95	—	1.89	—	3.16	—	3.91	—
Nonacosane	20.54	—	6.17	—	5.59	—	6.59	—	7.84	—	8.76	—
Triacontane	16.49	—	2.46	—	1.20	—	0.49	—	1.91	—	2.61	—
Hentriacontane	15.06	—	3.00	—	3.15	—	4.35	—	4.68	—	6.73	—
Dotriacontane	10.98	—	1.10	—	1.21	—	0.64	—	1.35	—	2.49	—
Tritriacontane	7.75	—	1.74	—	—	—	1.40	—	2.60	—	3.08	—

SOURCE: BRODDIN, et al. (1980)

Class III: Organics with clearly greater percent distribution in the gas phase (vapor pressure $> 1 \times 10^{-6}$ atm).

For alkanes this scheme leads to Class I ($>C_{24}$ alkanes), Class II (C_{18}-C_{24} alkanes) and Class III ($<C_{18}$ alkanes). Recent experimental studies on the volatilization of printing oils (C_{12}-C_{17} alkanes) show that once evaporated these materials stay in the gas phase (Battelle, 1982). Given the emission data provided by EPA for all chemicals of interest in this study, the atmospheric partial pressures shall be significantly lower than the vapor pressures in virtually all Class II and III cases. This concentration gradient in favor of vapor phase is further increased by the relatively high reactivity of many low volatility species (Appendix) leading to low partial pressures.

Although the above volatility guidelines for classification seem reasonable, we hasten to add that very little experimental data are available to draw rigorous boundaries under all atmospheric conditions. The experimental data are not only sparse but suffer from experimental artifacts. The Belgium studies (Broddin et al., 1980; Cautreels and Van Cauwenberghe, 1978) suffer from problems associated with retention of vapors as well as volatilization of aerosols during the process of sampling on filters. The nature of the aerosol itself could play a role in these artifacts. A true aerosol/vapor sampling system has not yet been devised. Nevertheless, the classification system proposed here is consistent with both qualitative as well as quantitative information available to date.

SECTION 4

DATA COLLECTION AND ESTIMATION

All data collected or estimated are summarized in the Appendix for each of the chemicals of interest. Since no measured data were available for a large number of chemicals, estimation methods had to be employed in such cases. All sources of data are cited and estimates clearly noted in the Appendix. In addition, comments are included that allow a better interpretation of these raw data. The overall process of data collection was divided into three categories. These are

- Smog chamber data (Reactivity)
- Measured rate constant data and rate constant estimation (Reactivity)
- Measured physical properties and their estimation (Volatility).

In the following sections, we shall briefly discuss these data. Complete details for individual compounds can be found in the Appendix.

SMOG CHAMBER DATA

These data provide the most direct determination of the O_3-forming ability of a chemical. Smog chamber data taken between 1959-present were found and employed in this study. All relevant references and important data are summarized in the Appendix. Most of the data are obtained with relatively low OC/NO_x ratios (2 to 10), and simulate irradiations of 3 to 7 hours. During the last decade, however, it has been increasingly felt that for chemicals of low reactivity, high OC/NO_x ratios (>20) and long irradiation times are conducive to high ozone formation. Some smog chamber data were available for approximately half of the 118 chemicals of interest. Although the sources of these data are many (Appendix), the following are some of the prominent ones:

- Stanford Research Institute (Schuck and Doyle, 1959)
- Los Angeles County (Brunelle et al., 1966)
- General Motors Research (Heuss and Glasson, 1968)
- Stanford Research Institute (Wilson and Doyle, 1970)
- Battelle Columbus Laboratories (Levy and Miller, 1970)
- Shell Oil Company (Laity et al., 1973)
- Bureau of Mines (Dimitriades et al., 1975)
- Rutgers University (Appleby, 1976)
- Environmental Protection Agency (Dimitriades and Joshi, 1977)
- MITI Japan (Yanagihara et al., 1977)
- Research Triangle Institute (Sickles et al., 1980)
- University of North Carolina (Jefferies et al., 1982)

The most important initial conditions and results from smog chamber irradiations are presented for each of the chemicals. A good deal of product analysis is also based on smog chamber studies. The identified products are summarized under comments in the Appendix. Where no product analysis is provided, it can be assumed that ozone, PAN and formaldehyde are the only identified products.

MEASURED RATE CONSTANT DATA AND RATE CONSTANT ESTIMATION

In the absence of any smog chamber data, reactivity of chemical species with hydroxyl (OH) radical provides a useful technique for establishing their involvement or noninvolvement in photochemical ozone formation. It is recognized that a direct and quantitative relationship between OH reactivity and ozone formation has not been established, and exceptions are known to exist. Nevertheless, available information provides strong support for the general validity of such relationships (Darnall et al., 1976; Winer et al., 1979; Akimoto and Sakamaki, 1983). In addition, these allow an independent assessment of the depletion rates measured in smog chambers, and indirectly, an estimation of the validity of experimental data. The exhaustive literature search was therefore conducted to collect measured OH-rate-constant data at 295-300^{o}K from the literature. These data and the relevant references are included in the Appendix. Two of the primary sources of OH rate constant data were compilations prepared by Atkinson et al. (1979) and Hampson (1980). Additional published and unpublished data for the period 1980-1983 were also sought and are cited. When applicable the rate constants with O_3 (for alkenes), and due to photolysis (aldehydes and ketones), are also included.

After an exhaustive survey of kinetic data, it became evident that the measured rates were available for only about 60% of the chemicals of interest. Thus, it was essential for us to estimate OH rate constants for the remainder of the chemicals. The method used was an updated version of the structure activity relationship (SAR) method developed by Hendry and Kenley (1979) and described by Davenport in Mill et al. (1982). This OH-rate-constant estimation technique included three major pathways for such reactions in the gas phase: (i) H-atom abstraction, (ii) addition to olefinic bonds and, (iii) addition to aromatic rings.

Each reaction path has an intrinsic reactivity constant for each reaction center, k_{ABST}, k_{OLEFIN}^{ADD}, and k_{AROM}^{ADD}. Each reactivity constant is modified by substituents on the reaction center (α-position) and adjacent to it (β-position), which are expressed as substituent constants α and β, respectively. Thus, the general expression for the OH SAR is

$$k_{OH} = k_{ABST} + k_{OLEFIN}^{ADD} + k_{AROM}^{ADD} \qquad (1)$$

$$k_{OH} = \sum_{i=1}^{p} n_i \, \alpha_{Hi} \, \beta_{Hi} \, k_{Hi} + \sum_{j=1}^{q} \alpha_{Ej} \, k_{Ej} + \sum_{l=1}^{r} \alpha_{A\ell} \, k_{A\ell} \qquad (2)$$

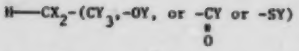
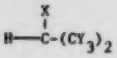
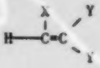
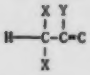
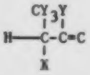
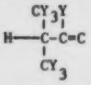
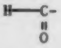
The term n_i is the number of times a structural group appears in the molecule. Each α_{Hi} is the product of α_H for each α-postion substituent (maximum of three for a methyl hydrogen). Likewise, each β_{Hi} is the product of β_H for the (up to nine) β-position substituents. The k_{Hi} term is the rate constant of the parent hydrocarbon group without substituents. Similarly α_{Ej} is the product of all substituent constants α_E for the substituents on the jth double bond while $\alpha_{A\ell}$ is the product of the substituent constants α_A for all substituents on a given aromatic ring (l). Each k_E or k_A is the rate constant for the double bond or aromatic structure type, respectively. Values of k, α and β are based on an extensive list of published rate constants for each kind of reaction or composite reaction constants that were divided into the contributory constants for each pathway. The current best values of these SAR constants are given in Tables 2 to 5 (from Davenport in Mill et al., 1982). For additional details on the application of these SAR constants, including examples, the reader is referred to Hendry and Kenley (1979), Mill et al. (1981) and Mill et al. (1982).

The validity of this OH reaction rate estimation method was tested for a set of approximately 100 chemicals for which the estimation technique is applicable and measured rate constants were available. Figure 8 shows these results for alkane, alkenes, haloalkenes, aldehydes, ethers, alcohols, acetates, ketones, sulfur compounds, aromatics, chlorobenzenes, and terpenes. For lack of available constants, the estimation methodology is not strictly applicable to alkynes, phthalates, nitrogenous compounds, and epoxides. It is clear from Figure 8 that the estimated rate constants in general are in agreement with measured values to within a factor of two (one standard deviation). For the purposes of this study, OH rate constants were estimated for those cases where no reliable measurement had been made. Occasionally, this was also used to suggest potential discrepancies in measured OH rate constants. The increase in scatter with decreasing rate constants in Figure 8 is due to less accurate measurements in this region. These also cause SAR constants to be less precise.

PHYSICAL PROPERTIES AND THEIR ESTIMATION

Literature data is relatively scarce for physical property information such as vapor pressure, solubility, or ambient phase distributions. The solubility of chemical in water can be estimated from the activity coefficient where the mole fraction of chemical in water is the inverse of the infinite dilution activity coefficient. Several methods are available for estimating

Table 2. Abstraction Rate Constants (k_H) for reactions of OH with generalized structures

Structure[*]	$10^{12}\ k_H$[**]
1. Primary carbon  $H-CX_2-(CY_3, -OY, \text{ or } -\underset{O}{\underset{\Vert}{C}}Y \text{ or } -SY)$	0.065 ± 0.013
2. Secondary carbon[†]  $H-\overset{X}{\overset{\vert}{C}}-(CY_3)_2$	0.55 ± 0.07
3. Tertiary carbon[†] $H-C-(CY_3)_3$	2.9 ± 0.58
4. Double bond[††]  $H-\overset{X}{\overset{\vert}{C}}=C\begin{smallmatrix}\diagup Y\\ \diagdown Y\end{smallmatrix}$	0.01 ± 0.002
5. Primary carbon, β-double bond[††]  $H-\underset{X}{\underset{\vert}{\overset{X}{\overset{\vert}{C}}}}-\overset{Y}{\overset{\vert}{C}}=C$	0.3 ± 0.1
6. Secondary carbon, β-double bond[††]  $H-\underset{X}{\underset{\vert}{\overset{CY_3}{\overset{\vert}{C}}}}-\overset{Y}{\overset{\vert}{C}}=C$	2.5 ± 1.0
7. Tertiary carbon, β-double bond[††]  $H-\underset{CY_3}{\underset{\vert}{\overset{CY_3}{\overset{\vert}{C}}}}-\overset{Y}{\overset{\vert}{C}}=C$	4.0 ± 1.5
8. Aldehyde[§]  $H-\underset{O}{\underset{\Vert}{C}}-$	17 ± 4
9. Mercaptan[§] $H-S-$	2.6 ± 1.3
10. Cresol $H-O-C$	1.7 ± 0.08

---

[*] The X's refer to α substituents, Y's to β substituents. The substituents are not necessarily identical. For example, Y's in $H-CX=CY_2$ could represent two different kinds of the substituent groups listed in Table 5; one Y may represent a Cl and the other an H. If no X or Y is listed, there is no substituent effect for that structure.

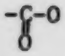
[**] Rate constant expressed as $cm^3\ molec^{-1}\ s^{-1}$.

[†] In addition to saturated carbon moieties, $\cdot CY_3$, $-OY$ $-\underset{O}{\underset{\Vert}{C}}-Y$ or $-S-Y$ moieties can be used instead as shown in structure 1.

[††] Olefinic or aromatic.

[§] No β substituents effects for these structures (i.e., $\beta_H = 1.0$ for all β structures).

Table 3. Induction factors for substituents[*]

Substituent, X or Y	α_H(for X's)	β_H(for Y's)
-H	1.0	1.0
-F	1.0	0.3 ± 0.1
-Cl	2.4 ± 0.5	0.4 ± 0.1
-Br	2.4 ± 0.05	0.4 ± 0.1
-OH	2.0 ± 0.05	1.0
-O-alkyl	6.0 ± 2.0	1.0
-C (alkyl)[†]	1.3 ± 0.2	1.0
 $-\underset{\overset{\|}{O}}{C}-O$	1.0	1.0
-N	100 ± 50	1.0
-S-	200 ± 100	1.0

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[*] See test for method of application and chapter by Davenport in Mill et al. (1982) for examples

[†] Only for structures 1 through 7, Table 2.

Table 4. Addition rate constants (k_E) for reaction of OH with carbon-carbon double bond and values of induction factors (α_E)

Substituent	$10^{12}k^*$ (per double bond)	Substituent α_E
none (ethene)	7.9	
1-alkyl	27.0 ± 5	H = 1.0
1,1-dialkyl	50.0 ± 10	F = 0.5 ± 0.3
cis-1,2-dialkyl	60.0 ± 12	Cl, Br = 0.7 ± 0.3
trans-1,2-dialkyl	70.0 ± 14	
trialkyl	80.0 ± 16	
tetraalkyl	150.0 ± 30	
vinyl or phenyl	80.0 ± 20	
methoxy	33.0	

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[*] Rate constant expressed as $cm^3\ molec^{-1}\ s^{-1}$.

Table 5. Addition rate constants (k_A) for reaction of OH with aromatic rings and values of induction factors (α_A)

Substituent	$10^{12} k_A$ *	Substituents	α_A
H	2.0 ± 0.6	H	1.0
Alkyl	5.0 ± 2	Cl	0.3
Dialkyl	12 ± 4	F,Br,I	< 1
1,2,3-Trialkyl	10 ± 5	--	--
1,2,4-Trialkyl	25 ± 5	--	--
1,3,5-Trialkyl	49 ± 5	--	--
Methoxy	17 ± 5	--	--
OH plus alkyl	34 ± 10	--	--
$-\underset{\underset{\displaystyle O}{\|}}{C}-H$	< 1.0	--	--

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[*] Rate constant expressed as cm^3 $molec^{-1}$ s^{-1}.

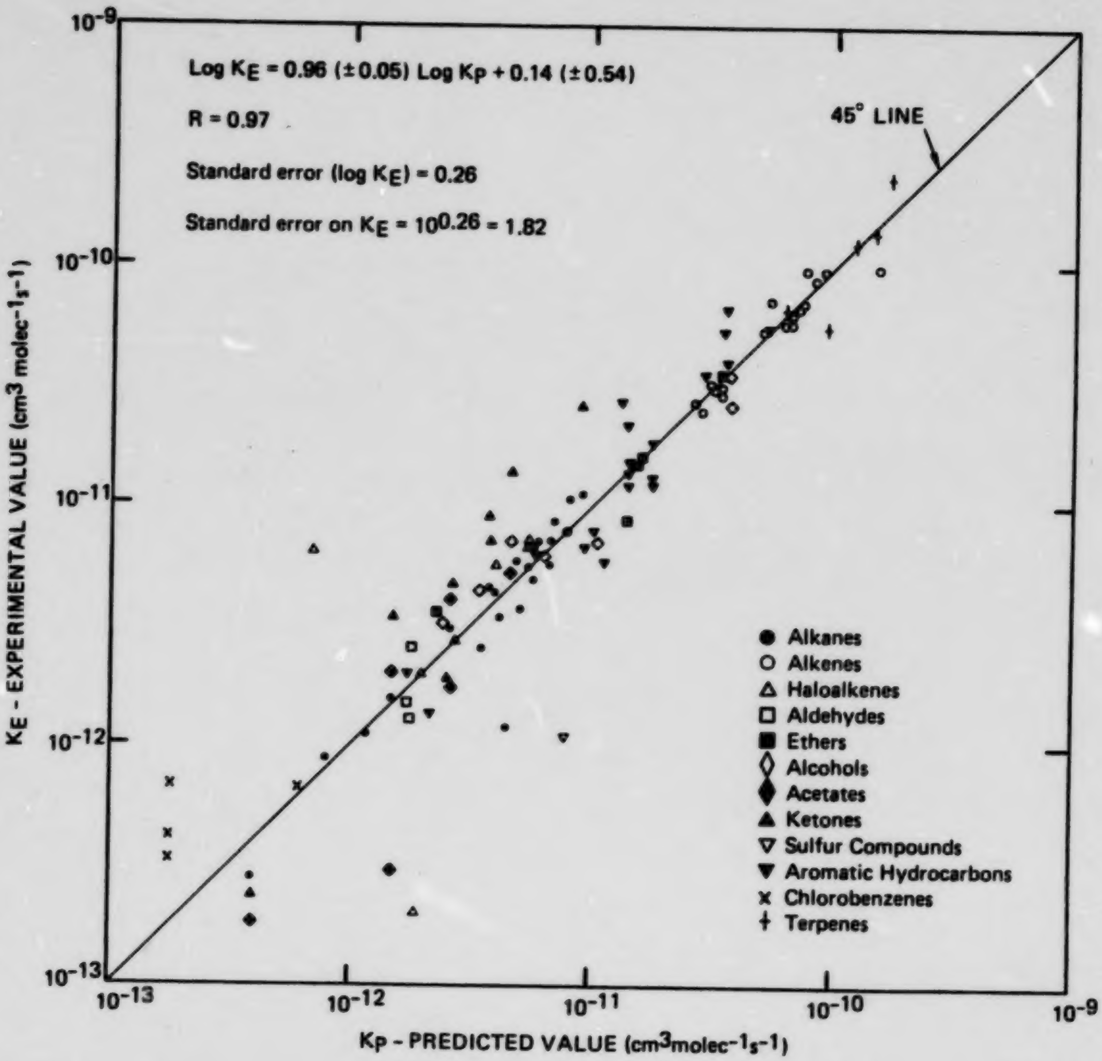


Figure 8. The relationship between predicted (K_p) and experimental (K_E) hydroxyl radical rate constants

the activity coefficients based solely on knowledge of the molecular structure. Correlation constants for an equation that considers contributions by solute and solvent functional groups and number of carbon atoms were developed by Pierotti et al., (1959), and are detailed in Lyman et al., (1982) and Reid et al., (1977).

Several correlation equations estimate vapor pressure from boiling and melting points. One recently reviewed method for estimating vapor pressures at below boiling point temperatures is described by Grain in Lyman et al.'s Handbook of Chemical Property Estimation Methods (1982). The method requires only the normal boiling point and is suitable for all organic materials over a wide pressure range. The Lyman method has a stated maximum error of 7.1% over the pressure range 0.01-1 atm, 50% between 1×10^{-6}-0.01 atm, and 200% below 1×10^{-6} atm. The average error is <50% which is often less than the range of vapor pressures found in the literature.

The Lyman method uses a modification of the Watson correlation to express the temperature dependence of ΔH_v such that

$$\Delta H_v \approx \Delta H_{vb} \left[3 - 2(T/T_B)\right]^m \qquad (3)$$

where ΔH_v is the heat of vaporization, ΔH_{vb} is the heat of vaporization at the normal boiling point, and m is a constant which depends upon the physical state. Substitution in the Clausius-Clapeyron equation and integration results in an expression with adjustable parameters that depend on the molecular structure and the physical state at the temperature of interest. With further modification, the Lyman method can also be used to estimate vapor pressures from boiling points at reduced pressure.

Henry's constants were calculated from the vapor pressure and solubility data given. A water solubility of 1.7×10^4 mol m^{-3} was used for chemicals which were completely miscible in water. Practically, the water solubility cannot exceed 10^{22} molecules/cm^3, since the molecular volume is > 10^{-22} cm^3 (Heicklen, 1981). This is equivalent to 1.7×10^4 mol m^{-3} at 25°C. For gaseous chemicals at 25°C, the convention is to calculate the Henry's constant for a total solute vapor pressure equal to one atmosphere because the solubility data is at atmospheric pressure. Chemicals with high solubility or in the gaseous state at ambient conditions will, therefore, not always have calculated values (Henry's constants) equal to the saturated vapor pressure divided by the solubility (P/C). In addition, the value on the data sheets may also differ from expected calculated values because of rounding off differences.

Henry's law is strictly applicable only to dilute solutions (mole fraction ≤ 0.001) and ideal gases where the activity coefficient is constant. For non-ideal systems, the activity is no longer constant and the solute vapor pressure exerted is smaller than for the pure solute. However, the magnitude of H for non-ideal systems can be used to broadly estimate environmental partitioning. In this study, it is assumed that most typical smog conditions occur during conditions of moderate-to-low humidity (<70% RH).

SECTION 5

REACTIVITY/VOLATILITY CLASSIFICATIONS AND DISCUSSION OF RESULTS

The raw data, as well as the reactivity, volatility, and overall classifications, are provided in the Appendix. To facilitate discussion these assigned classifications are summarized in Table 6. Shortcomings in data availability are also specified in this table. The overall classification utilizes the lowest rankings of the individual reactivity or volatility classification. We shall discuss the reasons, uncertainties, and shortcomings of individual rankings in the following sections.

CHEMICALS IN THE CLASS I CATEGORY

These chemicals are listed in Table 7. The reason for this designation (low reactivity or low volatility) is specified. Of the 26 chemicals ranked as Class I, only 4 are due to very low volatility. All of the nonreactive species have a reactivity less than that of ethane. Ethane, tested in a smog chamber under a variety of OC-to-NO_x ratio conditions, was found to yield no more than 0.08 ppm O_3 (Heuss, 1975). In the same study, propane yielded as much as 0.14 ppm O_3, suggesting that the NAAQS-O_3 level of 0.12 ppm corresponds to a reactivity level between those of ethane and propane. These data and comparisons are not unequivocal because of the questionable comparability of smog chamber and "real" atmospheres and of other uncertainties. However, in the lack of more definitive data, ethane is taken to be the best choice of "borderline" organic separating the "reactive" organics from the "unreactive" ones.

OH-rate-constants at 25°C relative to ethane vary from 0 to 1.0. In a number of instances (Chemical Nos. 6, 7, 25, 26, 28, 39, 48, 53, 54, 56, 71, 77, and 94), simulated laboratory irradiation data are available and show no O_3

Table 6. Reactivity/volatility classification of selected organic chemicals

Chemical Name	No.	Classification		
		Reactivity	Volatility	Overall
Acetic acid	1	III	III	III
Acetic anhydride	2	II[†]	III	II
Acetaldehyde	3	III	III	III
Acetone	4	III	III	III
Acetone cyanohydrin	5	II[†]	III	II
Acetonitrile	6	I	III	I
Acetylene	7	I	III	I
Acrylic acid	8	III[†]	III	III
Acrylonitrile	9	III	III	III
Adipic acid	10	III[†]	III	III
Aniline	11	II[*]	III	II
Benzene	12	II	III	II
Bisphenol-A	13	III[†]	I[**]	I
1,3-Butadiene	14	III	III	III
n-Butane	15	III	III	III
i-Butane	16	III	III	III
Butenes	17A-C	III	III	III
Isobutylene	18	III	III	III
n-Butanol	19	III	III	III
2-Butoxyethanol	20	III	III	III
n-Butyl acetate	21	III	III	III
s-Butyl acetate	22	III	III	III
t-Butyl alcohol	23	III	III	III
Carbon disulfide	24	II	III	II
Carbon tetrachloride	25	I	III	I
Chloroform	26	I	III	I
Monochlorobenzene	27	II	III	II
p-Dichlorobenzene	28	I	III	I
Dichloropropene (1,3 and 1,2)	29A-B	III[†]	III	III
Cumene	30	III	III	III
Cvclohexane	31	III	III	III
Cyclohexanol	32	III[†]	III	III
Cyclohexanone	33	III	III	III
Diethylene glycol	34	III[†]	III	III
Di-(2-ethylhexyl) phthalate	35	III[†]	I	I
Diisodecyl phthalate	36	III[†]	I	I
Dimethyl terephthalate	37	III[†]	III[**]	III
Epichlorohydrin	38	III[§]	III	III
Ethane	39	I	III	I
Ethanol amine (mono)	40A	III[†]	III	III
Ethanol amine (di)	40B	III[†]	I	I
Ethanol amine (tri)	40C	III[†]	II	II
Ethyl acetate	41	III	III	III
Ethyl alcohol	42	III	III	III
Ethyl benzene	43	III	III	III
Ethyl chloride	44	II[§]	III	II
2-Ethoxyhexanol	45	III[†]	III	III
Ethylene	46	III	III	III
Ethylene dibromide	47	I[§]	III	I
Ethylene dichloride	48	I	III	I
Ethyl ether	49	III	III	III
Ethylene glycol	50	III[†]	III	III
Ethylene oxide	51	I	III	I
2-Ethyl hexanol	52	III[†]	III	III
Fluorocarbon 11	53	I	III	I
Fluorocarbon 12	54	I	III	I
Fluorocarbon 22	55	I	III	I
Fluorocarbon 113	56	I	III	I
Fluorocarbon 114	57	I	III	I
Formaldehyde	58	III	III	III
Glycerine	59	II[†]	II	II
Hexamethylenetetramine	60	III[†]	II[**]	II
Heptenes	61	III	III	III
1,6-Hexane diamine	62	III[†]	III[**]	III

Table 6. (Continued)

Chemical Name	No.	Classification		
		Reactivity	Volatility	Overall
Hydrogen cyanide	63	I[§]	III	I
Isodecyl alcohol	64	III[†]	II	II
Isoprene	65	III	III	III
Isopropyl alcohol	66	III	III	III
n-Propyl alcohol	67	III[§]	III	III
Maleic anhydride	68	III[†]	III	III
Methanol	69	III	III	III
Methyl chloride	70	I[§]	III	I
Methylene chloride	71	I	III	I
Methyl ethyl ketone	72	III	III	III
Methyl isobutyl ketone	73	III	III	III
Methyl methacrylate	74	III	III	III
Solvent naphtha	75	III	III[**]	III
Naphthalene	76	II[*]	III	II
Nitrobenzene	77	I	III	I
n-Octyl-n-decylphthalate	78	III[†]	I	I
Nonylphenol (ethoxylated)	79	III[†]	II[††]	II
Perchloroethylene	80	I[*]	III	I
Phenol	81	II[*]	III	II
Phosgene	82	I[†]	III	I
Phthalic anhydride	83	III[†]	II	II
Propane	84	III	III	III
Propylene	85	III	III	III
Propylene glycol	86	III[†]	III	III
Propylene oxide	87	II[§]	III	II
Styrene	88	III	III	III
Terephthalic acid	89	III[†]	III	III
Terephthalic acid (dimethyl ester)	90,37	III	III[**]	III
Tetrapropylene	91	III[†]	III[**]	III
Toluene	92	III	III	III
Toluene diisocynate	93	III[†]	III	III
1,1,1-Trichloroethane	94	I	III	I
Trichloroethylene	95	III	III	III
Triethylene glycol	96	III[†]	III	III
Vinyl acetate monomer	97	III	III	III
Vinyl chloride monomer	98	III	III	III
m-and mixed Xylenes	99	III	III	III
o-Xylene	100	III	III	III
p-Xylene	101	III	III	III
Dimethyl succinate	102	III[†]	III[**]	III
Dimethyl glutarate	103	III[†]	III[**]	III
Dimethyl adipate	104	III[†]	III[**]	III
2-methoxy ethanol	105	III[†]	III[**]	III
Ethylene glycol monomethyl ether	106	III[†]	III	III
Ethylene glycol monoethyl ether	107	III[†]	III	III
Diisoamyl ketone	108	III[†]	II[††]	II
Propylene glycol methyl ether	109	III[†]	III	III
Dipropylene glycol methyl ether	110	III[†]	III	III
o,m,p Cresols	111A-C	III[§]	III	III

[†] No smog chamber or measured hydroxyl radical rate constant data were available.

[*] Exception requiring special interpretation of data (see text).

[**] Vapor pressure was estimated.

[§] No smog chamber data were available.

[††] No vapor pressure estimate was possible.

Table 7. Chemicals that may not participate in smog formation (Class I)

Chemical Name	NO.	Nonreactive	Nonvolatile	Comments*,†
Acetonitrile	6	✓		Significantly less reactive than ethane
Acetylene	7	✓		Reactivity comparable to ethane;
Bisphenol-A	13		✓	V.P. is 2 (-12) atm; very low partition coefficient. Highly reactive in gas phase
Carbon tetrachloride	25	✓		Unreactive in the troposphere
Chloroform	26	✓		Reactivity less than ethane
p-dichlorobenzene	28	✓		Reactivity comparable to ethane
Di-(2-ethyl hexyl) phthalate	35		✓	Vapor pressure is 2(-10) atm. Highly reactive in gas phase.
Diisodecyl phthalate	36		✓	V.P. is 4(-10) atm. Highly reactive in gas phase
Ethane	39	✓		Too unreactive to participate in smog formation
Ethanol amine (di)	40B		✓	V.P. is 2(-9) atm. Very low partition coefficient. Highly reactive in gas phase.
Ethylene dibromide	47	✓		Reactivity less than ethane
Ethylene dichloride	48	✓		Reactivity less than ethane
Ethylene oxide	51	✓		Less reactive than ethane
Fluorocarbon-11	53	✓		Unreactive in the troposphere
Fluorocarbon-12	54	✓		Unreactive in the troposphere
Fluorocarbon-22	55	✓		Significantly less reactive than ethane
Fluorocarbon-113	56	✓		Unreactive in the troposphere
Fluorocarbon-114	57	✓		Unreactive in the troposphere
Hydrogen cyanide	63	✓		Virtually unreactive in the troposphere
Methyl chloride	70	✓		Significantly less reactive than ethane
Methylene chloride	71	✓		Less reactive than ethane
Nitrobenzene	77	✓		Less reactive than ethane. Smog inhibitor
n-octyl-n-decyl phthalate	78		✓	V.P. is 9(-9) atm. Highly reactive in gas phase
Perchloroethylene	80	✓		Significantly less reactive than ethane
Phosgene	82	✓		Significantly less reactive than ethane
1,1,1-Trichloroethane	94	✓		Significantly less reactive than ethane

*2(-12) = 2 x 10^{-12}; V.P. = vapor pressure

†For additional discussions see Appendix and text.

Table 8. Estimation of average OH concentrations in three selected smog chambers

Chemical Name	No.	Measured OH rate constant, κ (cm^3 $molec^{-1}$ s^{-1})	Dimitriades and Joshi (1977)		Yanagihara et al. (1977)		Heuss and Glasson (1968)	
			Av. Disapp. rate DR (%/h)	$\overline{OH}$ (molec. cm^{-3})	Av. Disapp. rate DR (%/h)	$\overline{OH}$ (molec. cm^{-3})	Av. Disapp. rate DR (%/h)	$\overline{OH}$ (molec. cm^{-3})
Acetic acid	1	7.3(-13)*	2.0	7.6(6)§				
Acetonitrile	6	4.9(-14)	0.02††	1.1(6)				
Acetylene	7	1.7(-13)	6.3	1.0(8)	3.5	5.7(7)		
Acrylonitrile	9	4.1(-12)	5.3	2.3(6)				
Benzene	12	1.2(-12)	3.1	7.2(6)	3.3	7.6(6)	2.2	5.1(6)
n-Butane	15	2.7(-12)	1.4	1.4(6)	7.0	7.2(6)	0.8	0.8(6)
n-Butanol	19	7.6(-12)			7.4	2.7(6)		
n-Butylacetate	21	5.3(-12)†	4.3	2.3(6)	5.3	2.8(6)		
Chloroform	26	1.1(-13)	0.8	2.0(7)				
Monochlorobenzene	27	9.0(-13)			1.5	4.6(6)		
o-Dichlorobenzene	28†	2.5(-13)			4.3	4.8(7)		
Cumene	30	7.8(-12)					5.5	2.0(6)
Cyclohexane	31	6.2(-12)			5.8	2.6(6)		
Ethane	39	3.1(-13)	0.5	4.5(6)	11.0	9.8(7)		
Ethyl acetate	41	1.8(-12)			1.9	2.9(6)		
Ethyl alcohol	42	2.5(-12)			4.0	4.4(6)		
Ethyl benzene	43	8.0(-12)			6.5	2.3(6)	4.8	1.7(6)
1-Propanol	66	5.5(-12)	3.3	1.7(6)	4.0	2.0(6)		
Methanol	69	1.1(-12)	1.3	3.3(6)				
Methylene chloride	71	1.6(-13)	5.7	9.9(7)	1.9	3.3(7)		
Perchloroethylene**	80	1.7(-13)						
Propane	84	1.9(-12)	2.0	2.9(6)	4.1	5.9(6)		
Toluene	92	5.8(-12)			8.0	3.8(6)	6.5	3.1(6)
1,1,1-Trichloroethane	94	1.2(-14)	0.1††	2.3(7)				
Trichloroethylene	95	2.2(-12)			9.4	1.2(7)		
o-Xylene	100	1.2(-11)			11.1	2.6(6)	8.7	2.0(6)

Note: Initial Hydrocarbon (ppm) to NO_x (ppm) ratios are 4/0.2, 2/1 and 2/1 respectively for Dimitriades and Joshi (1977), Yanagihara et al. (1977) and Heuss and Glasson (1968).

*7.3(-13) = 7.3 x 10^{-13}. For source of rate constant data see Appendix.

†Rate measured for s-butyl acetate; No. 28 is p-dichloroberzene, the rate constant and measured depletion rates are for o-dichlorobenzene.

§$\overline{OH}$ = 2.78 x 10^{-6} (K^{-1}.DR)

**Not possible because of Cl atom reactions in smog chambers.

††In these experiments, disappearance rates of <0.1%/h are probably not quantitative.

formation above chamber background levels. In these and all other unreactive cases measured or estimated OH rate constants are utilized to arrive at Table 7.

Here we point out that even when smog chamber data are available for low reactivity chemicals, the results may be inapplicable. Table 8 summarizes the depletion rates from three smog chamber studies for those chemicals whose reactivity is exclusively with OH radicals and a measured OH-rate-constant is available. The estimated average OH values that prevailed in these smog chambers are listed in Table 8. Figure 9 shows a plot of the estimated OH concentration and the OH-rate-constant for each of the chemicals. Two salient observations can immediately be made from the results of Table 8 and Figure 9.

- The prevailing OH concentrations in a smog chamber can vary nearly 100-fold, depending upon the chemical being irradiated.
- The prevailing OH concentrations increase as the OH reactivity decreases.

It is also obvious from Figure 9 that this behavior is not limited to a single study. The best available estimates of OH abundance in the boundary layer of a polluted atmosphere is $3(\pm2) \times 10^6$ molec. cm^{-3} (Calvert, 1976; Singh et al., 1981). Therefore, we feel that smog chambers may not provide representative reactivity data for chemicals with an OH-rate-constant of less than $10^{-12} cm^3 molec^{-1} s^{-1}$, or roughly three times the rate constant for ethane. One reason for the prevailing high OH levels during such cases is the inability of low reactivity OCs to provide an effective OH removal process which are probably produced as a result of chamber wall effects. We hasten to add that the chemicals assigned Class I are less reactive than smog chamber experiments suggest, hence their classification will not change. On the other hand, some chemicals in Class II or III categories may more appropriately belong in Class I.

The four nonvolatile species in Class I category all have vapor pressures less than 10^{-8} atm and as low as 10^{-12} atm. All current experimental (Broddin et al., 1980) and theoretical evidence suggests that these compounds would be more than 75% partitioned in the particulate phase. In almost all of these cases, Henry's coefficients are also sufficiently low to favor the aerosol phase. We note, however, that all four of these species would be higly reactive if they

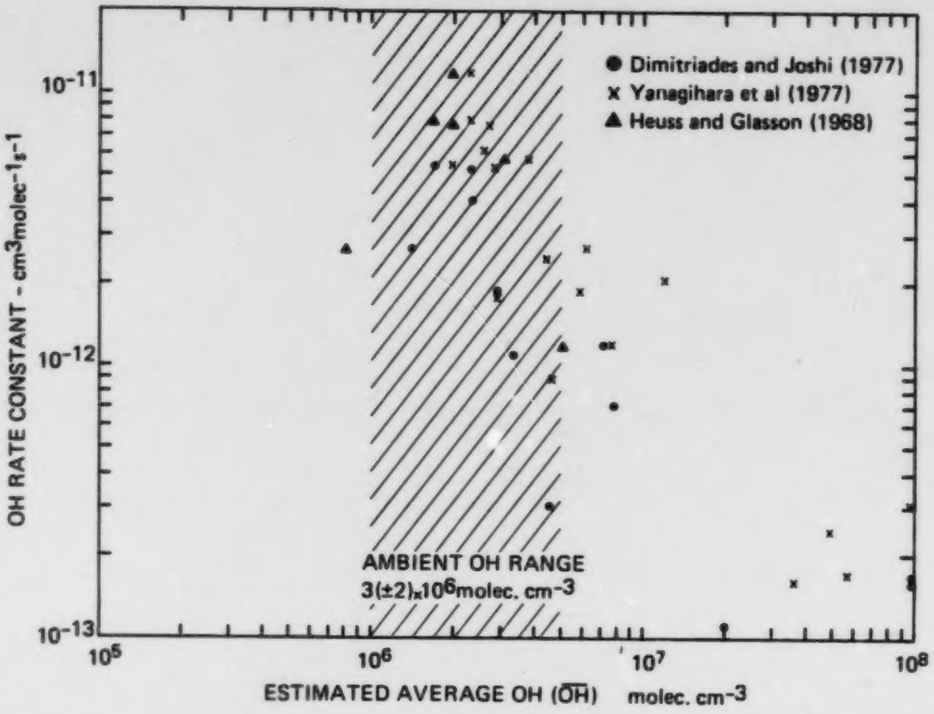


Figure 9. Relationship between OH rate constant and prevailing mean OH concentrations in three smog chambers

Table 9. Chemicals whose smog participation cannot be suitably defined (Class II)

Chemical Name	NO.	Intermediate Reactivity	Intermediate Volatility	Comments[*,†]
Acetic anhydride	2	✓		No S.C. or kinetic data; reactivity slightly greater than ethane
Acetone cyanohydrin	5	✓		No S.C. or kinetic data; reactivity slightly greater than ethane
Aniline	11			Reactive smog inhibitor, no S.C. data
Benzene	12	✓		
Carbon disulfide	24	✓		Insufficient and unreliable evidence of reactivity
Monochlorobenzene	27	✓		2 to 3 times as reactive as ethane
Ethanol amine (di)	40B		✓	V.P. is 7(-7) atm. Highly reactive in gas phase
Ethyl chloride	44	✓		No S. C. or kinetic data; reactivity slightly greater than ethane
Glycerine	59	✓	✓	About 5 times as reactive as ethane; V.P. = 3(-7) atm.
Hexamethylenetetramine	60		✓	V.P. is 8(-7) atm. Highly reactive in gas phase
Isodecyl alcohol	64		✓	V.P. is 8(-7) atm. Highly reactive in gas phase
Naphthalene	76			Reactive smog inhibitor, no S.C. data
Nonylphenol (ethoxylated)	79			No V.P. estimate possible
Phenol	81			Reactive smog inhibitor
Phthalic anhydride	83		✓	V.P. is 7(-7) atm. Low partition coefficient. Highly reactive in gas phase
Propylene oxide	87	✓		
Diisoamyl ketone	108			No V.P. estimate possible

[*] S.C. = smog chamber; V.P. = vapor pressure; 3(-7) = 3×10^{-7}

[†] For additional discussion see Appendix and text.

could exist in the gas phase (Table 7, Appendix). This is based on the assumption that the estimated rate constants are reliable

CHEMICALS IN THE CLASS II CATEGORY

Seventeen chemicals are designated as Class II (Table 9). Seven of these are in this category exclusively for reasons of moderate reactivity, and four for reasons of low volatility. One chemical (glycerine) is estimated to have low reactivity and low volatility, and for two other chemicals no vapor pressure estimate could be made. In addition, three chemicals are designated as Class II because they appear to behave exceptionally, and data are insufficient to draw definitive conclusions.

In general, compounds that are 1-to-5 times as reactive as ethane have been assigned to Class II, but there are some exceptions. Broadly speaking, this category reflects chemicals that are less reactive than propane, but more reactive than ethane. Some chemicals in this range have been assigned to Class III because smog chamber data show that these chemicals produce significant ozone. Specifically, acetic acid, butyl alcohol and methanol are 2.4, 2.0 and 3.5 times as reactive as ethane, respectively. The data of Dimitriades and Joshi (1977) and Sickles et al. (1980) support significant ozone formation for these three chemicals when the initial OC/NO_x ratio is >20. As discussed in the previous section, the validity of such smog chamber data can be subject to some question. In the absence of direct experimental evidence, species 1-to-5 times as reactive as ethane are designated Class II. Typically, reliable data showing significant ozone formation became available for species as reactive or more reactive than propane.

Other exceptions also exist. In the case of perchloroethylene, a variety of contradictory smog chamber data was available (Appendix). Because of the potential for high Cl atom concentrations in a smog chamber system, the data must be considered unrepresentative of atmospheric conditions. In the ambient troposphere, Cl atoms are virtually nonexistent and cannot participate in the kind of chemistry that exists within the smog chamber air mixture (Appleby, 1976; Gay et al., 1976). Recently, Dimitriades et al. (1983) reviewed this issue in more detail and concluded that perchloroethylene/NO_x smog chamber data cannot be extrapolated to ambient conditions. Based exclusively on OH reactivity, perchloroethylene is less reactive than ethane and may be assigned to Class I.

Carbon disulfide presents yet another anomalous case. The measured OH rate constant indicates negligible OH reactivity (Wine et al., 1980). The rate constant was measured in an inert atmosphere. There is unpublished evidence (private communication of S. Penkett, Harwell, U.K.) that in an oxygen atmosphere the OH rate constant is much faster. Smog chamber data of Sickles and Wright (1979) show significant loss rate (1 to 4% hourly loss rate) but high ozone is produced only in one case when the initial CS_2/NO_x ratio is 20. When this ratio is 2, 4, and 10, no significant ozone formation occurs. In all cases however, carbonyl sulfide and sulfur dioxide were identified as products. Until more conclusive information is generated, carbon disulfide is assigned to Class II.

In addition, some chemicals that are more than five times as reactive as ethane have been placed in Class II because they behave exceptionally. The cases of aniline, naphthalene, and phenol are noted. The OH-based reactivity of these chemicals is more than 50 times that of ethane (Appendix). Limited smog chamber runs for aniline and naphthalene (Spicer et al., 1974) show a good deal of aerosol formation, but no ozone is produced. Similarly, phenol irradiations fail to show significant O_3 formation (Sickles et al., 1980). It is likely that the inability of benzene to produce ozone (Table 9, Appendix) is directly linked with the fact that phenol consitutes a dominant product of benzene photooxidation (Hendry, 1979). Chemicals, such as aniline, naphthalene, and phenol are well known free-radical scavengers, and have been tested in laboratories as candidate chemicals that could inhibit smog formation (Gitchell et al., 1974; 1974a). There is evidence for one inhibitor (Diethylhydroxyl amine) which suggests that under appropriate conditions even inhibitors can produce large concentrations of ozone (Pitts et al., 1979; Cupitt and Corse, 1979). Additional studies are needed to further elucidate the involvement of these species in the processes of smog formation which prevail under more typical atmospheric conditions.

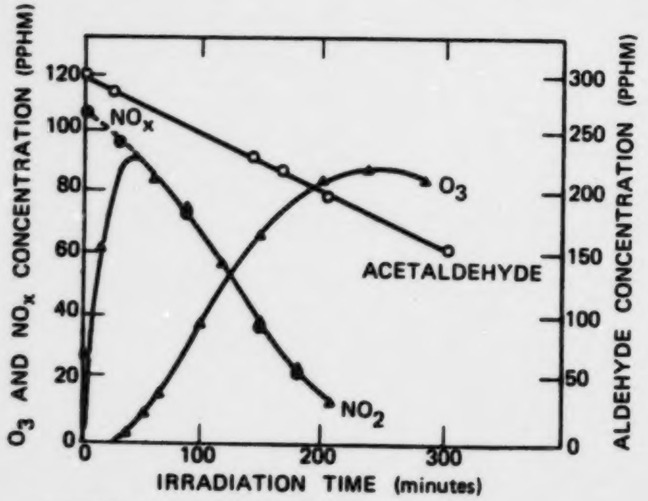
The species of intermediate volatility (10^{-6}-10^{-8} atm vapor pressure) are also listed in Table 9. Except for glycerine, which is only moderately reactive, all of the moderate volatility chemicals would be highly reactive if they could exist in the gas phase (Table 9, Appendix). This assumes that the estimated OH rate constants are a reliable indicator of reactivity.

CHEMICALS IN THE CLASS III CATEGORY

Of the 118 chemicals investigated during this study, 75 are designated as Class III, i.e., chemicals that are sufficiently volatile and reactive to participate in smog formation. To be included in this category, the following conditions were met:

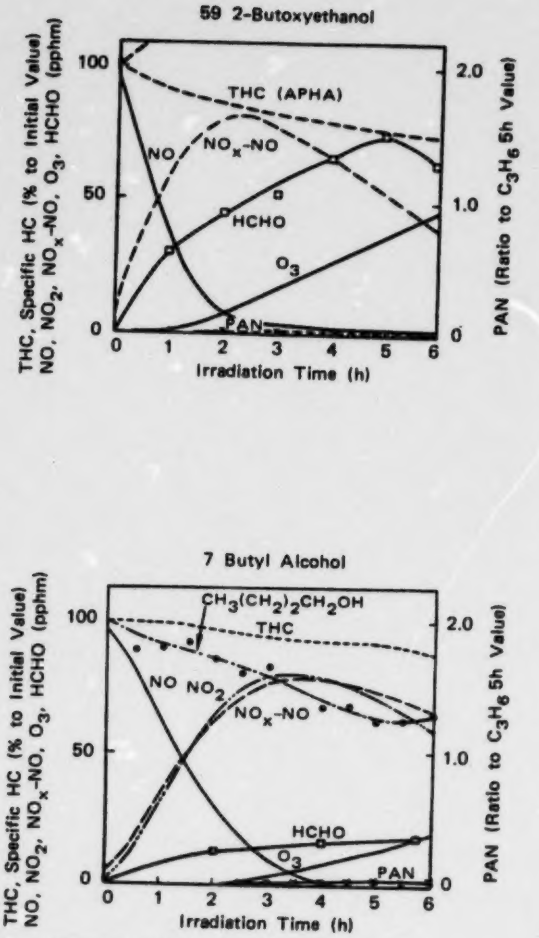
- Smog chamber data (OC concentration ≤ 4 ppm and any NO_x concentration) showed significant ozone formation (≥ 0.12 ppm).
- In the absence of smog chamber data, the chemical was at least 5 times as reactive as ethane. [Although OH reactivity is most important, photolysis as well as reactions with other species (O_3, O^{3P}, NO_3) were considered when applicable.]
- No significant reasons existed to disregard available smog chamber or kinetic data.
- The vapor pressure was greater than 10^{-6} atm (25°C), and Henry's coefficients were moderate-to-high.

We emphasize that good and representative smog chamber data were available for several chemicals to allow us to conclude that, in general, chemicals which show OH-based reactivity of greater than five times that of ethane can produce significant ozone concentrations. Propane, which is about six times as reactive as ethane, is one case where substantial evidence for ozone production exists. As stated earlier, acetic acid, t-butyl alcohol, and methanol are only 2-to-4 times as reactive as ethane even though smog chamber data show significant ozone formation (Dimitriades and Joshi, 1977; Sickles et al., 1980). Here we point out that measured OH-rate constants have been published for only methanol, although an unpublished measurement was available for acetic acid. Additionally, highly reactive chemicals, such as toluene diisocyanate and cresols, may act as smog inhibitors by terminating free radical chains. Little conclusive evidence on the role of inhibitors is available in the literature. Diethylhydroxyl amine (DEHA), a known free radical scavenger, has been shown to produce significant ozone (Pitts et al., 1977; Cupitt and Corse, 1979). The reason for classification III selection for individual chemicals (Table 6) is self-explanatory. All the data as well as comments dealing with mechanisms, data availability, and product analysis can be found in the Appendix. A number of these chemicals have already been measured in the ambient gas phase (Brodzinsky and Singh, 1982) and are known to exist in the gas phase in the chamber atmospheres (Appendix). Figures 10-14 show results of smog chamber irradiations for a wide variety of structurally different compounds. In all these cases, significant ozone concentrations are encountered. These chemicals include oxygenated species such as aldehydes and alcohols (Figures 10 and 11), 1-heptene (Figure 12), toluene (Figure 13), and the naturally-occurring isoprene (Figure 14). It should also be pointed out that even the relative ozone-forming potential of a reactive species is dependent on many variables including the OC/NO_x ratio and the chemical composition of the mixture (Bufalini and Dodge, 1983).



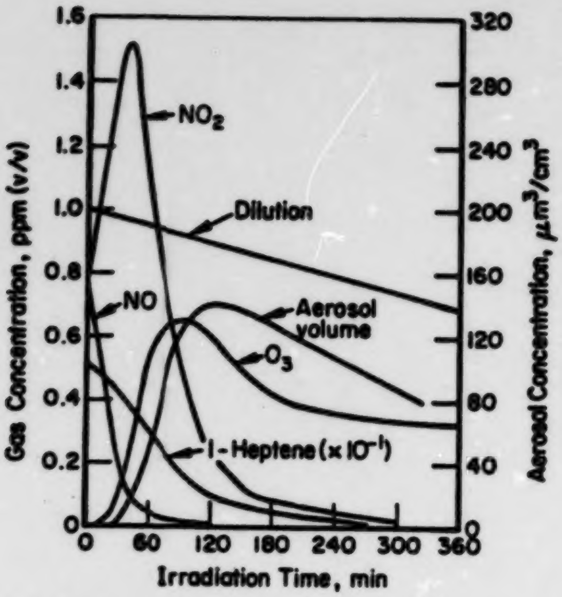
SOURCE: KUNTZ, et al. (1973)

Figure 10. Irradiation of acetaldehyde-NO_x-air-photochemical system



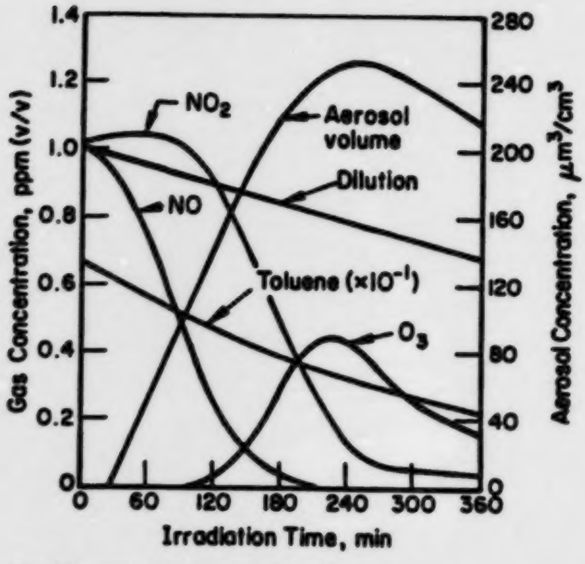
SOURCE: YANAGIHARA, et al. (1977)

Figure 11. Smog chamber irradiations of 2-Butoxyethanol and Butyl alcohol in a NO_x-air system



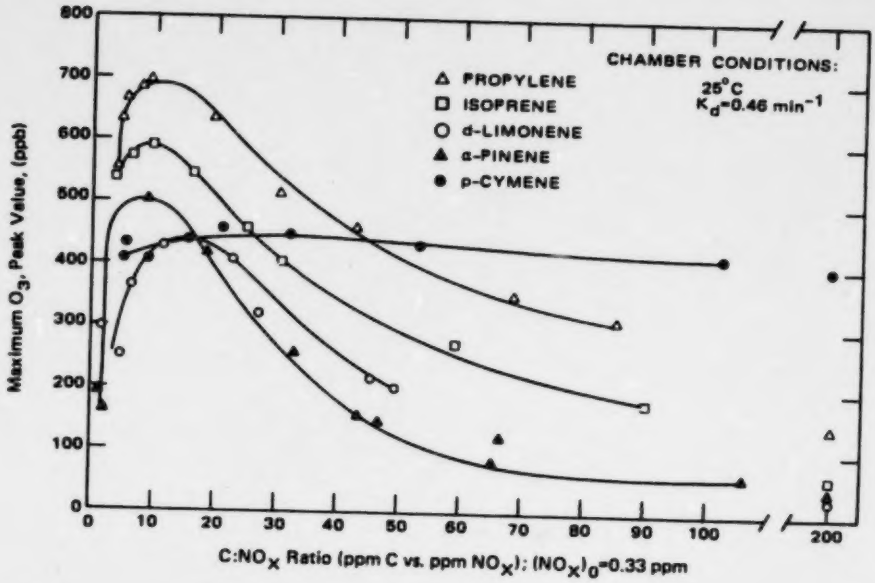
SOURCE: MILLER AND JOSEPH, (1976)

Figure 12. Smog chamber irradiation of a 1-Heptene-NO$_x$-air mixture



SOURCE: MILLER AND JOSEPH, (1976)

Figure 13. Smog chamber irradiation of a Toluene-NO$_x$-air mixture



SOURCE: ARNTS, et al.(1981)

Figure 14. Maximum ozone formation as a function of OC to NO_x ratio for some biogenic chemicals and propene

SECTION 6

RECOMMENDATIONS

For a sizable fraction of the 118 chemicals for which reactivity/volatility classifications were sought, a severe absence of data was evident. Smog chamber irradiations had been performed for only half of the chemicals of interest. Hydroxyl radical rate constants had been measured for about 60% of the chemicals. The situation with volatility parameters (vapor pressure and partition coefficients) was also not dissimilar.

It is clear, therefore, that even preliminary experimental data are lacking for a sizable fraction of the chemicals of interest. Further, for those cases where some data are available, considerable judgment was needed because of the inadequacy of the data. Thus, while we have used our best possible judgments based on available information, the need for additional theoretical and experimental studies is overwhelming. In the following sections, we discuss several specific as well as general shortcomings.

1. The ozone-forming ability of hydrocarbons is known to be dependent on the initial OC/NO_x ratio (e.g., Figures 3 and 4). The OC/NO_x ratio that leads to maximum O_3 formation is a function of the reactivity of the species (Figure 4). It is clear that the lesser the reactivity, the greater the OC/NO_x ratio that leads to maximum O_3 production. Much of the smog chamber irradiation data are available at an OC/NO_x ratio of 2-to-5 with some studies operating at a ratio of 20. We feel that smog chamber irradiations should be performed at a number of OC/NO_x ratios, with at least one irradiation at a ratio suggested by Figure 4. Additional data are needed to develop a more comprehensive

Figure 4. For many chemicals of moderate-to-low reactivity, existing smog chamber evidence obtained at an OC/NO_x ratio of about 2 and showing no O_3 formation, is misleading.

2. Analysis of smog chamber data shows that the OH radical concentrations (a key to smog initiation processes) vary widely from run to run. A 100-fold variability in OH concentrations can be justified from available data. It further appears that the discrepancies are most severe (highest OH levels) for the least reactive chemicals (Table 5, Figure 9). This raises serious questions about the atmospheric applicability of smog chamber data for chemicals with OH radical reaction rate constants of $<10^{-12}$ cm^3 $molec^{-1}$ s^{-1} (Figure 9). The reason may be the inability of these less-reactive chemicals to provide an effective sink mechanism for OH removal. Smog chamber wall effects may also dominate the photochemical system. Therefore, we recommend that irradiations of such low-reactivity species be performed in mixture with more reactive chemicals. In such cases, the OH rate constant, when available, can provide a better means for extrapolating to ambient conditions compared with smog chamber data.

3. As a routine practice all smog chamber runs should be spiked with trace quantities of a known chemical which can be independently monitored to infer OH concentrations. This is particularly important for low-reactivity chemicals since only a small fraction may react, leading to large errors in measuring depletion rates. A suggested chemical for such an OH-tracer application is trichloroethylene. At an initial concentration of 1 part per billion (ppb) in chamber experiments, it can be monitored accurately for several hours. At this low concentration, it is not likely to perturb ongoing chemistry (e.g., via cl atoms) in a smog chamber with precursors present at three orders of magnitude higher concentrations. Alternatively, 5 to 10 ppb of propane or n-butane may also be an adequate OH tracer. For these suggested tracers, ozone reactions are too slow to be significant. Since most smog chamber runs are performed at 1-to-4 ppm reactant concentrations, the system is negligibly perturbed.

4. The classification system developed in this study would not have been possible without our ability to predict OH radical rate constants. Although

tests with experimental data (Figure 8) are highly encouraging, these predictive capabilities should be further developed and expanded. Currently, the predictive technique used here is not strictly applicable to chemicals such as alkynes, nitrogenous compounds, epoxides, and phthalates. This is largely due to the unavailability of constants on which these structure-activity relationships are based. There is a great need to expand and further develop these predictive capabilities.

5. As a category, organic acids have been studied least of all. Except for acetic acid, no kinetic or smog chamber data were available for any of the acids. Even for acetic acid, the OH-rate constant data have not yet been published and may be in error.

6. A number of highly reactive free radical scavengers (such as naphthalene) do not appear to form O_3 even though they lead to high aerosol production. The smog chamber data of this class of inhibitors (phenols, naphthalene, nitrobenzene, aniline and possibly cresols) are too scarce to be meaningful. Tentative evidence exists to support the contention that at least some of these inhibitors may produce ozone upon prolonged irradiations. Irradiations at both low and high OC/NO_x ratios need to be performed to further ascertain their photochemical role.

7. For a number of chemicals, smog chambers do not simulate the ambient atmosphere. Perchloroethylene, due to its complex Cl initiated chemistry, is one such known chemical. Trichloroethylene and other halogenated chemicals can be expected to behave similarly. Neither their O_3-forming ability nor the product distribution can be easily extrapolated from smog chambers to ambient conditions. Such shortcomings of smog chamber experiments should be identified in as many cases as possible.

8. A reliable, parallel, aerosol/gas sampling system does not exist. Vaporization of particulate matter and condensation of vapors is known to occur when samples are collected on a variety of filters. The development of a true aerosol/gas sampling system is urgently needed.

9. The available data base on ambient partitioning of chemicals is very scarce. Atmospheric variables (such as temperature, humidity, particulate loading and particulate composition) affect partitioning to different degrees, but correlations do not exist to estimate the relative importance of these factors. A large body of data may allow volatility estimates with a lot more confidence than is possible today.

10. For a wide variety of nonvolatile materials, the vapor pressure data are either not available, or must be extrapolated over large temperature ranges. This shortcoming can be dealt with only when determinations are made for vapor pressure under ambient type conditions.

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Appendix

REACTIVITY/VOLATILITY DATA SHEETS AND CLASSIFICATIONS FOR 118 SELECTED SPECIES*

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*The quantity in parenthesis is raised to the power of 10 $7.3(-13)=7.3\times10^{-13}$. All the properties are at room temperature (25°C) unless otherwise specified. When necessary, OH rate constants and vapor pressure data were estimated by methods of Hendry and Kenley (1979) and Lyman et al. (1982) as described in the text. Henry's constants were estimated from vapor pressure and solubility data as described in the test. Inf. (infinite) means the chemical is miscible in the solvent in all proportions. To obtain Henry's coefficient in dimensionless form (C_{gas}/C_{liq}) multiply by 41.0.

Chemical Name: Acetic acid

Chemical NO.: 1

Chemical Formula: CH_3COOH (M.W.=60)

CAS Registry NO.: 64-19-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.42		10-12			Sickles et al (1980)
4.0	0.07	0.25	0.94		10-12			Sickles et al (1980)
4.0	0.2		0.26	13.7		2.0		Dimitriades and Joshi (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.3 (-13)	Zetzsch (1983)	2.4	Unpublished data
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.1 (-2)	Dreisbach (1961)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Dreisbach (1961)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	1.2 (-6)		calculated
SOLVENT SOLUBILITY (mol. m^{-3})	miscible	Merck (1976)	alcohol, carbon tetrachloride, glycerol, ether, carbon disulfide
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Smog chamber data shows acetic acid reactivity to be consistent with an OH radical concentration of $8x10^6$. This seems much too high. Acetic acid has been measured in the ambient air in gas phase (Dawson et al., 1980).

Chemical Name: Acetic anhydride

Chemical NO.: 2

Chemical Formula: $(CH_3CO)_2O$(M.W.=102)

CAS Registry NO.: 108-24-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3					
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)	TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.0 (-13)	Estimated	1.3	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.7 (-3)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	1900		Estimated
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.5 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	Chloroform, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II

VOLATILITY: III

OVERALL: II

E. GENERAL COMMENTS

Acetic anhydride is not likely to undergo gas phase hydrolysis and thus can participate as an intact molecule in smog chemistry. In contact with water droplets rapid hydrolysis to acetic acid occurs. Although SAR suggest an OH rate constant of $4x10^{-13}$, it also suggests a relative rate of 2 times the acetic acid rate. Thus, a value of $1.4x10^{-12}$ could also be inferred leading to Reactivity Classification III.

Chemical Name: Acetaldehyde

Chemical NO.: 3

Chemical Formula: CH_3CHO (M.W.=44)

CAS Registry NO.: 75-07-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.4	0.25	0.94		10-12			Jefferies et al (1982)
0.5	0.5	0.37	0.60		10-12	8.0		Kamens et al (1981)
3.0	1.0	0.0	0.90	4.0	5	10.0	30.0	Kuntz et al (1973)
1.0	0.5	0.14	0.71		6		13.7	Dimitrades and Wesson (1972)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.5 (-11)	Atkinson et al (1979)	48.4	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}	1.0 (-5)	Hendry et al (1980)		

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2	Jordan (1954)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	inf.	Verschueren (1977)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	6 (-5)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	alcohol
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Acetaldehyde is nearly as effective in O_3 formation as propylene (Cox et al, 1980). Photochemical reaction products such as formaldehyde, carbon monoxide, peroxyacetyl nitrate, methyl nitrate, and hydrogen peroxide have been identified.

Chemical Name: Acetone

Chemical NO.: 4

Chemical Formula: $(CH_3)_2CO$ (M.W.=58)

CAS Registry NO.: 67-64-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3					
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)	TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
4.7	0.24	0.40	0.02		10-12			Jefferies et al (1982)
4.0	0.2	0.25	0.49		10-12		1.5 propane	Sickles et al (1980)
4.0	0.2		0.18	12.1		0.9		Dimitriades and Jashi (1977)
2.0	1.0	0.05	0.0		5	0.0	1.5	Yanagihara et al (1977)
1.5	0.6	0.05	0.1 x toluene		5	≈2	0.2 x toluene	Laity et al (1973)
4.0	2.0	0.0			6	0.0		Levy and Miller (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.0 (-13)	Cox et al (1980)	1.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}	5.0 (-6)	Calvert and Pitts (1966)		

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.6 (-1)	Weast (1973)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	inf.	Freier (1975)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	1.6 (-5)		calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	alcohol, chloroform, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

The very high OC/NO_x ratios lead to significant O_3 formation. Moderate or low OC/NO_x ratios show no O_3 formation. Kinetic considerations show reactivity with photolysis playing a dominant role.

Chemical Name: Acetone Cyanohydrin

Chemical NO.: 5

Chemical Formula: $(CH_3)_2C(OH)CN$ (M.W.=85)

CAS Registry NO.: 75-86-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.0 (-13)	Estimated	1.9	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-3)		Estimated
WATER SOLUBILITY (mol. m^{-3})	3900		Estimated
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.2 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	insoluble	Merck (1976)	Carbon disulfide, petroleum ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** III **OVERALL:** II

E. GENERAL COMMENTS

No laboratory or smog chamber data are available.

Chemical Name: Acetonitrile

Chemical NO.: 6

Chemical Formula: CH_3CN (M.W.=41)

CAS Registry NO.: 75-05-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.01		10-12			Sickles et al (1980)
4.0	0.07	0.25	0.01		10-12			Sickles et al (1980)
4.0	0.2		0.0	31		0.02		Dimitriades and Joshi (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.9 (-14)	Harris et al (1981)	0.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	$\leq$1.5 (-19)	Harris et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.1 (-1)	Dreisbach (1961)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	6.6 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	Methanol, acetone, chloroform, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Significantly less reactive than ethane.

Chemical Name: Acetylene

Chemical NO.: 7

Chemical Formula: C_2H_2 (M.W.=26)

CAS Registry NO.: 74-86-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.15		10-12		0.9xpropane	Sickles et al (1980)
4.0	0.07	0.25	0.15		10-12		0.9xpropane	Sickles et al (1980)
4.0	0.2		0.10	5.3		6.3		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	3.4	2.8	Yanagihara et al (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.7 (-13)	Atkinson et al (1979)	0.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	8.6 (-20)	NAS (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	48	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	29	Stephen and Stephen (1963)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	3.4 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	1050 990 720	Miyano and Hayduk (1981)	benzene methanol Hexane
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

The high disappearance rates cannot be reasonably explained. These would require prevailing OH concentrations of approximately 10^8 molec cm^{-3} which are much too high. The Sickles et al (1980) data may suffer from high background O_3 levels. These smog chamber data are inconsistent with our current knowledge of photochemistry.

Chemical Name: Acrylic acid

Chemical NO.: 8

Chemical Formula: $CH_2CHCOOH$ (M.W.=72)

CAS Registry NO.: 79-10-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.8 (-11)	Estimated	90.3	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.3 (-3)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.2 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Expected to be significantly more reactive than acetic acid.
No smog chamber or laboratory kinetic data are available.

Chemical Name: Acrylonitrile

Chemical NO.: 9

Chemical Formula: CH_2CHCN (M.W.=53)

CAS Registry NO.: 107-13-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	1.9		10-12		2xpropane	Sickles et al (1980)
4.0	0.07	0.25	1.1		10-12		2xpropane	Sickles et al (1980)
4.0	0.2		0.37	5.5		5.3		Dimitriades and Joshi (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.1 (-12)	Harris et al (1981)	13.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	≤1.0 (-19)	Harris et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.5 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	1500	Lyman et al (1982)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	9.8 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Adipic acid

Chemical NO.: 10

Chemical Formula: $HOOC(CH_2)_4COOH$ (M.W.=146)

CAS Registry NO.: 124-04-9

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	4.4 (-12)	Estimated	14.2	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.3 (-4)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	137	Morrison and Boyd (1973)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.5 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	acetone, methanol, ethanol
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.
Should be significantly more reactive than acetic acid.

Chemical Name: Aniline

Chemical NO.: 11

Chemical Formula: $C_6H_5NH_2$ (M.W.=93)

CAS Registry NO.: 62-53-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.8	0.96		0.0		4			Spicer et al (1974)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2(-10);2.4(-11)	Gusten et al (1981); Barnes et al (1982)	387.1 to 77.4	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.8 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	390	Dreisbach (1955)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	2.2 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	benzene, alcohol, chloroform
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II

VOLATILITY: III

OVERALL: II

E. GENERAL COMMENTS

Although highly reactive, it is a known smog inhibitor (Gitchell et al, 1974). It does, however, contribute significantly to aerosol formation (Spicer et al, 1974).

Chemical Name: Benzene

Chemical Formula: C_6H_6 (M.W.=78)

Chemical NO.: 12

CAS Registry NO.: 71-43-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.02	1.5		3.1		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	3.3	1.9	Yanagihara et al (1977)
1.0	0.5	0.11	0.0		6		1.1-1.6	Dimitriades et al (1975)
1.5	0.6	0.05	0.2x toluene		5	≈2.4	0.2xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.0		6			Levy and Miller (1970)
2.0	1.0	0.05	0.05		6	2.2	1.6	Heuss and Glasson (1970)
8.0	2.0	0.0	0.0		6			Brunelle et al (1966)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-12)	Atkinson et al (1979)	3.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.3 (-1)	Zwolinski and Wilhoit (1971)	
WATER SOLUBILITY (mol. m^{-3})	22.8	McAuliffe (1966)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	5.4 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, acetone, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** III **OVERALL:** II

E. GENERAL COMMENTS

Although moderately reactive, it is inefficient in ozone formation. A large fraction of products (≈100%) is phenol (Hendry, 1979). This radical scavenger may be responsible for preventing significant O_3 formation.

Chemical Name: Bisphenol-A

Chemical NO.: 13

Chemical Formula: $HOC_6H_4-C(CH_3)_2-C_6H_4OH$ (M.W.=228)

CAS Registry NO.: 80-05-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.0 (-11)	Estimated	225.8	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.9 (-12)		Estimated
WATER SOLUBILITY ($mol.\ m^{-3}$)	1.5 (-1)	Freier (1975)	20°C
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	1.2 (-11)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	soluble slightly soluble	Merck (1976)	alcohol, acetone carbon tetrachloride
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** I **OVERALL:** I

E. GENERAL COMMENTS

No laboratory or smog chamber data are available.

Chemical Name: Butadiene-1,3 **Chemical NO.:** 14

Chemical Formula: $CH_2CHCHCH_2$ (M.W.=54) **CAS Registry NO.:** 106-99-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.79	1.8	5	20.0	23.1	Yanagihara et al (1977)
1.0	0.5	0.11	0.89		6		13.0	Dimitriades et al (1975)
1.0	0.4	0.05			7		4.3	Glasson and Tuesday (1970)
2.0	1.0	0.05	0.48		6	15.0	25.0	Heuss and Glasson (1968)
3.3	0.85		0.72		3	27.5		Altshuller et al (1966)
3.0	1.0	>20	0.65	0.75	6	49.0		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.9 (-11)	Atkinson et al (1979)	222.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	8.4 (-18)	Niki (1978)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.77	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	13.6	McAuliffe (1966)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	7.4 (-2)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Highly reactive. Several photochemical products including formaldehyde, acrolein, nitric acid, peroxyacetyl nitrate, ethyl nitrate, propionaldehyde, acetone, and propylene oxide have been identified.

Chemical Name: n-Butane

Chemical NO.: 15

Chemical Formula: $CH_3CH_2CH_2CH_3$ (M.W.=58)

CAS Registry NO.: 106-97-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.1	0.55	0.27	0.16		10-12			Jefferies et al (1982)
2.0	1.0	0.05	0.05		5	7.0	4.0	Yanagihara et al (1977)
7.4	0.2	0.05	0.22		10	1.4		Zfonte and Bonamassa (1977)
4.0	0.2		0.23		12	1.4		Dimitriades and Joshi (1977)
1.0	0.5	0.11	0.04		6		1.8	Dimitriades et al (1975)
3.0	0.3		0.7		6	2.5		Altshuller and Bufalini (1971)
6.0	0.6		0.9		6	2.0		Altshuller and Bufalini (1971)
2.0	1.0	0.05	0.16		6	0.8	4.6	Heuss and Glasson (1968)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.7 (-12)	Atkinson et al (1979)	8.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.0 (-23)	NAS (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.4	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	1.1	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.5 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	1.9 (4)	Gerrard (1976)	Octanol
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Ozone formation is highly sensitive to initial HC/NO_x ratio. A ratio of 5 to 10 is most efficient in O_3 formation. A number of photochemical products such as acetaldehyde, carbon monoxide, carbon dioxide, methyl ethyl-ketone, formaldehyde, peroxyacetyl nitrate, methyl nitrate, ethyl nitrate, propylnitrate, butylnitrates, and butyraldehyde have been identified.

Chemical Name: Iso-Butane

Chemical NO.: 16

Chemical Formula: $(CH_3)_2CHCH_3$ (M.W.=58)

CAS Registry NO.: 75-28-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1	0.4	0.05					0.6	Glasson and Tuesday (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.4 (-12)	Atkinson et al (1979)	7.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	2.0 (-23)	NAS (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.4	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	8.4 (-1)	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.2	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Reactivity should be very nearly identical to n-Butane. Rate of NO_2 formation for i-Butane is also comparable to n-Butane (0.60 vs. 0.75) and is roughly twice as much as propane (Glasson and Tuesday, 1970).

Chemical Name: 1-Butene

Chemical NO.: 17A

Chemical Formula: $CH_3CH_2CHCH_2$ (M.W.=56)

CAS Registry NO.: 106-98-9

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.57	4.8	5	19.0	11.8	Yanagihara et al (1977)
1.0	0.5	0.11	0.67		6		7.0	Dimitriades et al (1975)
2.0	1.0	0.05	0.47		6	14.0	13.0	Heuss and Glasson (1968)
1.2	0.8	0.14	0.43		6			Brunelle et al (1966)
3.0	1.0	>20	0.58	0.75	3	55.0		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.9 (-11)	Atkinson et al (1979)	93.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-17)	Niki (1979)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.9	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	4.0	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.6 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Highly reactive chemical (Stephens and Burleson, 1967; Altshuller and Bufalini, 1971). Known products include formaldehyde, acetaldehyde, propionaldehyde, carbon monoxide, peroxyacetyl nitrate, peroxypropionyl nitrate, nitric acid, butyraldehyde, butylene oxide, methyl nitrate, ethyl nitrate, ethane and ethene.

Chemical Name: cis-2-Butene

Chemical NO.: 17B

Chemical Formula: $CH_3CHCHCH_3$ (M.W.=56)

CAS Registry NO.: 590-18-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.5	0.11	0.74		6		23.5	Dimitriades et al (1975)
2.0	1.0	0.05	0.44		6	15.0	28.0	Heuss and Glasson (1968)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.3 (-11)	Atkinson et al (1979)	138.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.4 (-16)	Niki (1979)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.1	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	1.4	Lyman et al (1982)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	7.1 (-1)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: trans-2-Butene

Chemical NO.: 17C

Chemical Formula: $CH_3CHCHCH_3$ (M.W.=56)

CAS Registry NO.: 624-64-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.5	0.14	0.70		6		34.1	Dimitriades et al (1975)
4.0	2.0	0.0	0.67	0.8	6		82.6	Levy and Miller (1970)
2.0	1.0	0.05	0.44		6	7.1	38.0	Heuss and Glasson (1968)
3.0	1.0	> 20	0.73	0.5	3	50.0		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	6.8 (-11)	Atkinson et al (1979)	219.4	
O_3	$cm^3 molec^{-1} s^{-1}$	2.6 (-16)	Niki (1979)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.3	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	1.4	Lyman et al (1982)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	7.1 (-1)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Known reaction products include: acetaldehyde, peroxyacetyl nitrate, carbon monoxide, formaldehyde, methyl ethyl ketone, methyl nitrate and nitric acid.

Chemical Name: Isobutylene

Chemical NO.: 18

Chemical Formula: $(CH_3)_2CCH_2$ (M.W.=56)

CAS Registry NO.: 115-11-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.75	2.0	6	20.0	15.6	Yanagihara et al (1977)
1.0	0.4	0.05					3.5	Glasson and Tuesday (1970)
5.0	3.0	0.0					80.0	Altshuller and Cohen (1963)
3.0	1.0	>20	1.0	0.5	1.7	55.0	-20.0	Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.7 (-11)	Atkinson et al (1979)	151.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	6.0 (-18)	Niki (1979)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.0	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	4.7	McAuliffe (1966)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	2.1 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Highly reactive. NO oxidation ability comparable to propene (Glasson and Tuesday, 1970).

Chemical Name: n-Butanol

Chemical NO.: 19

Chemical Formula: $C_3H_7CH_2OH$ (M.W.=74)

CAS Registry NO.: 71-36-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.28	13.8		1.1		Dimitriades and Joshi (1977)*
2.0	1.0	0.05	0.14		5	7.4	5.7	Yangihara et al (1977)
1.0	0.6	0.05	1.4x toluene		5	≈9.6	1.0xtoluene	Laity et al (1973)
1.0	0.1	2.7	0.13		7	9.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.6 (-12)	Atkinson et al (1979)		
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.4 (-3)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	1000	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	8.1 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

*These data are for t-Butanol which is less reactive than n-butanol (Laity et al, 1973)

Chemical Name: 2-Butoxyethanol

Chemical NO.: 20

Chemical Formula: $C_4H_9OCH_2CH_2OH$ (M.W.=119)

CAS Registry NO.: 111-76-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.38		5	4.5	9.3	Yanagihara et al (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.6 (-11)	Estimated	51.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.4 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	423	Merck (1976)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.9 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: n-Butyl acetate

Chemical NO.: 21

Chemical Formula: $CH_3COOC_4H_9$ (M.W.=116)

CAS Registry NO.: 123-86-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.02		5	5.3	3.5	Yanagihara et al (1977)
4.0	0.2		0.18	4.3		4.3		Dimitriades and Joshi (1977)*
1.0	0.6	0.05	0.8x toluene		5	4.4	0.7xtoluene	Laity et al (1973)
4.0	2.0	0.0	>0.08		6		6.0	Levy and Miller (1970)*
1.0	0.2	5.3	0.11		7	5.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.3 (-12)	Atkinson et al (1979)	16.1	Rate assumed to be the same as that of s-Butyl acetate
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.4 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	43	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	3.3 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Ethyl acetate at high OC/NO_x ratios (Sickles et al, 1980) shows significant O_3 formation. Butyl acetate should be at least as much or more reactive than ethyl acetate.

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*These data are for i-Butyl acetate

Chemical Name: sec-Butyl alcohol **Chemical NO.:** 22

Chemical Formula: $C_2H_5CHOHCH_3$ (M.W.=74) **CAS Registry NO.:** 78-92-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.6	0.05	1.3x toluene		5		1.0xtoluene	Laity et al (1973)
1.0	0.1	1.5	0.13		7	6.0		Wilson and Doyle (1970)*

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.3 (-12)	Estimated	23.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.2 (-2)	Jordan (1954)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	1700	Morrison and Boyd (1973)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	1.3 (-5)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

*These data are for iso-Butyl alcohol.

Chemical Name: t-Butyl alcohol

Chemical NO.: 23

Chemical Formula: $(CH_3)_3COH$ (M.W.=74)

CAS Registry NO.: 75-65-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.28	13.8		1.1		Dimitriades and Joshi (1977)
1.0	0.6	0.05	0.3x toluene		5	≈ 2	0.3xtoluene	Laity et al (1973)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.0 (-13)	Estimated	1.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.5 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Frier (1975)	$20^{\circ}C$
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.3 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Carbon disulfide

Chemical NO.: 24

Chemical Formula: CS_2 (M.W.=76)

CAS Registry NO.: 75-15-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	0.98	0.25	0.0		10	1.4		Sickles and Wright (1979)
2.0	0.49	0.25	0.01	8.6	10	2.2		
2.0	0.20	0.25	0.05	8.1	10	2.8		
2.0	0.10	0.25	0.33	9.3	10	3.8		

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	<1.5 (-15)	Wine et al (1980); WMO (1982)	≈0.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				
O		3.4 (-12)	WMO (1982)		

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.8 (-1)	Dreisbach (1961)	
WATER SOLUBILITY (mol. m^{-3})	22	Freier (1975)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.2 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	methanol, ether, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** III **OVERALL:** II

E. GENERAL COMMENTS

OH rate constant is negligible. However, there is enough evidence to suggest that in the presence of oxygen it may be much faster. Assuming an O(3p) concentration of $4x10^4$molec. cm^{-3}, no significant reactivity occurs. Excited state Cs_2 oxidation (Wine et al., 1980) may lead to some SO_2 production but the kinetics are not well understood. Smog chamber data show considerable reactivity, but cannot be considered firm. COS and SO_2 are key secondary products.

Chemical Name: Carbon tetrachloride

Chemical NO.: 25

Chemical Formula: CCl_4 (M.W.=154)

CAS Registry NO.: 56-23-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.05	0.5		0.0		200	0.0		Lillian et al (1975)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	<1.0 (-16)	Hampson (1980)	≈ 0.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.5 (-1)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	7.5	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.0 (-2)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	(1976)	alcohol, benzene, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I

VOLATILITY: III

OVERALL: I

E. GENERAL COMMENTS

Completely unreactive in the troposphere. Decomposition by photolysis occurs in the stratosphere (WMO, 1982).

Chemical Name: Chloroform

Chemical NO.: 26

Chemical Formula: $CHCl_3$ (M.W.=119)

CAS Registry NO.: 67-66-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.02		10-12		0.4xpropane*	Sickles et al (1980)
4.0	0.07	0.25	0.2		10-12		0.8xpropane*	Sickles et al (1980)
4.0	0.2		0.0	2.4		0.8		Dimitriades and Joshi (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.1 (-13)	Hampson (1980)	0.35	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.6 (-1)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	78	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.8 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, benzene, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I

VOLATILITY: III

OVERALL: I

E. GENERAL COMMENTS

Reactivity expected to be significantly less than ethane. At very high OC/NO_x ratios (≈50) O_3 production is seen (Sickles et al, 1980). However, high background O_3 levels may be responsible for this observation.

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*Maximum rate of NO oxidation.

Chemical Name: Monochlorobenzene

Chemical NO.: 27

Chemical Formula: C_6H_5Cl (M.W.=113)

CAS Registry NO.: 108-90-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.0		5	1.5	1.7	Yanagihara et al (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.0 (-13); 9.0 (-13)	Gusten et al (1981); Mill et al (1982)	1.6-2.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.5 (-2)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	4.4	Dreisbach (1955)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.8 (-3)	Mackay et al (1979)	
SOLVENT SOLUBILITY (mol. m^{-3})	freely soluble	Merck (1976)	alcohol, benzene, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** III **OVERALL:** II

E. GENERAL COMMENTS

Only about half as reactive as benzene. Irradiations with high OC/NO_x ratio have not been performed. Should behave similarly to benzene.

Chemical Name: p-Dichlorobenzene

Chemical NO.: 28

Chemical Formula: 1,4-$C_6H_4Cl_2$ (M.W.-147)

CAS Registry NO.: 106-46-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.02	3.5	5	4.3	3.9	Yanagihara et al (1977)*

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.5 (-13)	Mill et al (1982)	0.8	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.3 (-3)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	5.4 (-1)	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.3 (-3)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, benzene, ether
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

*Data are for o-dichlorobenzene. The measured smog chamber depletion rate is much too fast.

Chemical Name: 1,3-Dichloropropene

Chemical NO.: 29A

Chemical Formula: $CH_2ClCHCHCl$ (M.W.=111)

CAS Registry NO.: 542-75-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.3 (-11)	Estimated	41.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.3 (-2)		Estimated
WATER SOLUBILITY (mol. m^{-3})	63		Estimated
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	6.8 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: 1,2-Dichloropropene

Chemical NO.: 29B

Chemical Formula: $CH_3CClCHCl$ (M.W.=111)

CAS Registry NO.: 563-54-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.3 (-11)	Estimated	41.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.3 (-1)		Estimated
WATER SOLUBILITY (mol. m^{-3})	16		Estimated
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	7.9 (-3)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Cumene (Isopropylbenzene) **Chemical NO.:** 30

Chemical Formula: $C_6H_5CH(CH_3)_2$ (M.W.=120) **CAS Registry NO.:** 98-82-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.5	0.11	0.28		6		4.0	Dimitriades et al (1975)
4.0	2.0	0.0	0.41	5.3	6		6.5	Levy and Miller (1970)
2.0	1.0	0.05	0.19		6	5.5	6.6	Heuss and Glasson (1968)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.8 (-12)	Atkinson et al (1979)	25.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.1 (-3)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	4.2 (-1)	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.3 (-2)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Cyclohexane

Chemical NO.: 31

Chemical Formula: C_6H_{12} (M.W.=84)

CAS Registry NO.: 110-82-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.09		5	5.8	5.0	Yanagihara et al (1977)
4.0	2.0	0.0	0.27*	6.0	6		11.0	Levy and Miller (1970)
3.0	1.0	>20	0.20	1.4	3	45		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	6.2 (-12)	Atkinson et al (1979)	20.0	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.3 (-1)	Zwolinski and Wilhoit (1971)	
WATER SOLUBILITY (mol. m^{-3})	6.5 (-1)	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.8 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	ethanol, acetone, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

*O_3 still increasing at the end of the run.

Chemical Name: Cyclohexanol

Chemical NO.: 32

Chemical Formula: $C_6H_{11}OH$ (M.W.=100)

CAS Registry NO.: 108-93-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.6 (-12)	Estimated	21.3	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.7 (-3)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	360	Verschueren (1977)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.7 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	ethanol, aromatic hydrocarbons
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Cyclohexanone **Chemical NO.:** 33

Chemical Formula: $C_6H_{10}O$ (M.W.=98) **CAS Registry NO.:** 108-94-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.08	5.0	5	6.2	6.4	Yanagihara et al (1977)
1.0	0.6	0.05	0.6x toluene		5	4.0	0.8xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.10	4.8	6		8.5	Levy and Miller (1970)
1	0.2	1.2	0.08		7	7.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	5.5 (-12)	Estimated	17.7	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.8 (-3)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	230	Verschueren (1977)	20°C
HENRY'S CONSTANT (atm. $m^3 mol^{-1}$)	2.5 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Irradiation at high OC/NO_x ratios have not been performed.

Chemical Name: Diethylene glycol

Chemical NO.: 34

Chemical Formula: $HOCH_2CH_2OCH_2CH_2OH$ (M.W.=106)

CAS Registry NO.: 111-46-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.7 (-12)	Estimated	8.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.5 (-6)		Estimated
WATER SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	5.6 (-10)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf. insoluble	Merck (1976)	alcohol, acetone, ether benzene, carbon tet.
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Di-(2-ethylhexyl)phthalate

Chemical NO.: 35

Chemical Formula: $C_{24}H_{38}O_4$ (M.W.=390)

CAS Registry NO.: 117-81-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.8 (-11)	Estimated	90.3	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.9 (-10)	Klopffer et al (1982)	
WATER SOLUBILITY (mol. m^{-3})	1.0 (-4)	Klopffer et al (1982)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.9 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** I **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name: Diisodecyl phthalate

Chemical NO.: 36

Chemical Formula: $C_6H_4(COOC_{10}H_{21})_2$ (M.W.=447)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.4 (-11)	Estimated	109.7	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.8 (-10)		Estimated from boiling point data
WATER SOLUBILITY ($mol.\ m^{-3}$)			
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)			
PHYSICAL STATE			

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: I

OVERALL: I

E. GENERAL COMMENTS

Chemical Name: Dimethyl terephthalate

Chemical NO.: 37

Chemical Formula: p-$CH_3OOCC_6H_4COOCH_3$ (M.W.=194)

CAS Registry NO.: 120-61-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	1.2 (-11)	Estimated	38.7	Not strictly amenable to estimation
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.0 (-3)		Estimated from boiling point data
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	solid		

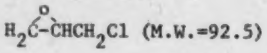
D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Epichlorohydrin

Chemical NO.: 38

Chemical Formula: 
$H_2\overset{O}{C}-CHCH_2Cl$ (M.W.=92.5)

CAS Registry NO.: 106-89-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.4 (-11)	Dilling et al (1976)	77.4	These data show that the relative loss rate of epichlorohydrin and 1,1,2 trichloroethane are identical. Rate constant used is that of the latter.
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.1 (-2)	Jordan (1954)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	650	Verschueren (1977)	20°C
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	3.2 (-5)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Ethane

Chemical NO.: 39

Chemical Formula: C_2H_6 (M.W.=30)

CAS Registry NO.: 74-84-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.03	3.0		0.5		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	11.0	3.0	Yanagihara et al (1977)
2.0	1.0	0.05	0.0		6	0.0		Farley (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	3.1 (-13)	Hampson (1980)	1.0	
O_3	$cm^3 molec^{-1} s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	38.5	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	2.0	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	5.0 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	825 535 215	Wilhelm and Battino (1973)	Benzene Acetone Methanol
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

The involvement of ethane in photochemical reactions is not in doubt (Singh and Hanst, 1981) but it is considered too unreactive to participate in smog formation (Singh et al, 1981). Over a 24 hr period no reactivity is observed by Stephens and Burleson (1967). High depletion rates measured by Yanagihara et al (1977) can only be explained as a smog chamber artifact.

Chemical Name: Ethanol amine

Chemical NO.: 40A

Chemical Formula: $OHCH_2CH_2NH_2$ (M.W.=61)

CAS Registry NO.: 141-43-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.3 (-11)	Estimated	41.9	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.2 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20^oC
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.2 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	777 inf.	Merck (1976)	benzene acetone
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Somewhat more reactive than diethylamine. The latter has been irradiated in smog chambers (0.5 ppm Oc/0.25 ppm NO_x) and produced significant ozone concentrations (Pitts et al, 1978).

Chemical Name: Diethanol amine

Chemical NO.: 40B

Chemical Formula: $(OHCH_2CH_2)_2NH$ (M.W.=105)

CAS Registry NO.: 111-42-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.3 (-11)	Estimated	138.7	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.1 (-9)		Estimated
WATER SOLUBILITY ($mol.\ m^{-3}$)	9100	Verschueren (1977)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	1.3 (-13)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	233 444	Merck (1976)	benzene ether
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** I **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name: Triethanol amine **Chemical NO.:** 40C

Chemical Formula: $(OHCH_2CH_2)_3N$ (M.W.=149) **CAS Registry NO.:** 102-71-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.0 (-11)	Estimated	129.0	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.2 (-7)		Estimated
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.3 (-11)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	2300 900	Merck (1976)	benzene ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** II **OVERALL:** II

E. GENERAL COMMENTS

Chemical Name: Ethyl acetate

Chemical NO.: 41

Chemical Formula: $CH_3COOC_2H_5$ (M.W.=88)

CAS Registry NO.: 141-78-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.80		10-12		1.8xpropane	Sickles et al (1980)
4.0	0.07	0.25	0.65		10-12		1.2xpropane	Sickles et al (1980)
2.0	1.0	0.05	0.01		5	1.9	2.6	Yanagihara et al (1977)
1.0	0.6	0.05	0.8x toluene		5	2.4	0.5xtoluene	Laity et al (1973)
1.0	0.2	0.7	0.08		7	4.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	1.8 (-12)	Atkinson et al (1979)	5.8	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	843	Stephen and Stephen (1963)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.4 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, acetone, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Reactivity comparable to propane. High OC/NO_x ratios are required to produce significant ozone formation.

Chemical Name: Ethyl alcohol **Chemical NO.:** 42

Chemical Formula: C_2H_5OH (M.W.=46) **CAS Registry NO.:** 64-17-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.64		10-12		1x propane	Sickles et al (1980)
4.0	0.07	0.25	0.73		10-12		1x propane	Sickles et al (1980)
2.0	1.0	0.05	0.0		5		2.2	Yanagihara et al (1977)
1.0	0.6	0.05	1xtoluene		5	≈ 2.8	2.6xtoluene	Laity et al (1973)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	2.5 (-12)	Atkinson et al (1979)	8.1	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.8 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20^oC
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.6 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Ethyl benzene

Chemical NO.: 43

Chemical Formula: $C_6H_5CH_3$ (M.W.=106)

CAS Registry NO.: 100-41-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.24		5	6.5	5.4	Yanagihara et al (1977)
1.0	0.5	0.11	0.32		6		4.2	Dimitriades et al (1975)
1.0	0.6	0.05	1xtoluene		5	6.4	0.8xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.42		6		10.9	Levy and Miller (1970)
2.0	1.0	0.05	0.21		6	4.8	7.2	Heuss and Glasson (1968)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	8.0 (-12)	Atkinson et al (1979)	25.8	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-2)	Zwolinski and Wilhoit (1971)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	1.4	McAuliffe (1966)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	7.9 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Chemical Name: Ethyl chloride **Chemical NO.:** 44

Chemical Formula: C_2H_5Cl (M.W.= 64.5) **CAS Registry NO.:** 75-00-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.9 (-13)	Hampson (1980)	1.3	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.58	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	89	Verschueren (1977)	20°C
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	1.1 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	8500	Merck (1976)	alcohol
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name: 2- Ethoxy hexanol

Chemical NO.: 45

Chemical Formula: $C_2H_5OCH_2CH_2OC_2H_5$ (M.W.=118)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.8 (-12)	Estimated	15.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-3)	Verschueren (1977)	
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Chemical Name: Ethylene

Chemical NO.: 46

Chemical Formula: C_2H_4 (M.W.=28)

CAS Registry NO.: 74-85-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	0.6	0.50	1.1		10-12			Jefferies et al (1982)
2.0	1.0	0.05	0.44	5.0	5	11.3	9.6	Yanagihara et al (1977)
1.8	0.8	>20	1.2	4.0	4	21.0		Gay et al (1976)
2.1	1.0	0.0	0.9	5.0	6	14.0		Gay et al (1976)
1.0	0.5	0.11	0.56		6		4.1	Dimitriades et al (1975)
4.0	2.0	0.0	0.59	4.0	6		24.0	Levy and Miller (1970)
2.0	1.0	0.05	0.28		6	7.5	5.8	Heuss and Glasson (1968)
6.0	2.0	>20	1.0	2.3	3	35.0		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	7.9 (-12)	Atkinson et al (1979)	25.4	
O_3	$cm^3 molec^{-1} s^{-1}$	1.8 (-18)	Niki (1979)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	59.9	Zwolinski and Wilhoit (1971)	
WATER SOLUBILITY (mol. m^{-3})	4.7	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.2 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	680 605 240	Wilhelm and Battino (1973)	benzene acetone methanol
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Products are acetaldehyde, formaldehyde, PAN, carbon monoxide, ethylene oxide and methyl nitrate.

Chemical Name: Ethylene dibromide

Chemical NO.: 47

Chemical Formula: CH_2BrCH_2Br (M.W.=188)

CAS Registry NO.: 106-93-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.5 (-13)	Hampson (1980)	0.81	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.5 (-2)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	27		Estimated
HENRY'S CONSTANT (atm. m^3 mol^{-1})	5.7 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name:	Ethylene dichloride	**Chemical NO.:**	48
Chemical Formula:	CH_2ClCH_2Cl (M.W.=99)	**CAS Registry NO.:**	107-06-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.08		10-12		0.5xpropane	Sickles et al (1980)
4.0	0.07	0.25	0.45		10-12		0.8xpropane	Sickles et al (1980)
1.0	0.2				400	≈0		Appleby (1976)*

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	2.2 (-13)	Hampson (1980)	0.7	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.1 (-1)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	88	Dilling (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.1 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether, chloroform
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Sickles et al (1980) were able to see O_3 levels as high as 0.22 ppm in the absence of NO_x ($OC/NO_x=\infty$). The O_3 value measured by Sickles is suspect.

*plus 0.5 ppm gasoline mixture

Chemical Name: Ethyl ether

Chemical NO.: 49

Chemical Formula: $C_2H_5OC_2H_5$ (M.W.=74)

CAS Registry NO.: 60-29-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.6	0.05	2.5xtoluene		5	12.0	1.7xtoluene	Laity et al (1973)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	8.9 (-12)	Atkinson et al (1979)	28.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.1 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	816	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	8.7 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	benzene, pet. ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Ethyl ether is about 50% more reactive than toluene based on OH reactivity alone.

Chemical Name: Ethylene glycol

Chemical NO.: 50

Chemical Formula: CH_2OHCH_2OH (M.W.=62)

CAS Registry NO.: 107-21-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	4.4 (-12)	Estimated	14.2	
O_3	$cm^3 molec^{-1} s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.7 (-4)	Short et al (1983)	
WATER SOLUBILITY ($mol. m^{-3}$)	inf.	Merck (1976)	
HENRY'S CONSTANT ($atm. m^3 mol^{-1}$)	1.0 (-8)		Calculated
SOLVENT SOLUBILITY ($mol. m^{-3}$)	inf. insoluble	Merck (1976)	acetone benzene, petr. ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

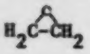
OVERALL: III

E. GENERAL COMMENTS

Should be about 50% more reactive than ethanol.

Chemical Name: Ethylene oxide

Chemical NO.: 51

Chemical Formula: 

H_2C-CH_2 (M.W.=44)

CAS Registry NO.: 75-21-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	2.0	0.11	< 0.01		53			Joshi et al (1982)
4.0	2.0	0.11	0.03		53			Joshi et al (1982)
4.0	0.2	0.25	0.02		10-12		0.5xpropane	Sickles et al (1980)
4.0	0.07	0.25	0.08		10-12		0.5xpropane	Sickles et al (1980)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.10^{-14}	Gusten et al (1981)	0.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.72	Conway et al (1983)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Conway et al (1983)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	5.9 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

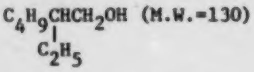
REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name: 2-Ethyl hexanol

Chemical NO.: 52

Chemical Formula:



$C_4H_9CHCH_2OH$ (M.W.=130) with C_2H_5 on the CH

CAS Registry NO.: 104-76-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.0 (-11)	Estimated	32.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.8 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	67.6	Lyman et al (1983)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.1 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Fluorocarbon-11

Chemical NO.: 53

Chemical Formula: $CFCl_3$ (M.W.=137)

CAS Registry NO.: 75-69-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3					
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)	TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
0.012	0.5		0.0		400	0.0		Lillian et al (1975)
0.025*	1.0				7	0.0		Hester et al (1974)
0.025†					1400	0.0		Hester et al (1974)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	<1.0 (-17)	Hampson (1980)	0.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.08	DuPont (1969)	
WATER SOLUBILITY (mol. m^{-3})	8.0	DuPont (1969)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.2 (-1)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Unreactive in the troposphere (WMO, 1982)

*plus 1 ppm C_4H_8

†in ambient air

Chemical Name: Fluorocarbon-12

Chemical NO.: 54

Chemical Formula: CCl_2F_2 (M.W.=121)

CAS Registry NO.: 75-71-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.02	0.5				400	0.0		Lillian et al (1975)
0.008*	1.0				7	0.0		Hester et al (1974)
0.025†					1440	0.0		Hester et al (1974)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	< 1.0 (-16)	Hampson (1980)	0.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.53	DuPont (1969)	
WATER SOLUBILITY (mol. m^{-3})	2.3	DuPont (1969)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.3 (-1)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I

VOLATILITY: III

OVERALL: I

E. GENERAL COMMENTS

Unreactive in the troposphere

*plus 1 ppm C_4H_8

†in the ambient air

Chemical Name: Fluorocarbon-22

Chemical NO.: 55

Chemical Formula: $CHClF_2$ (M.W.=86.5)

CAS Registry NO.: 75-45-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.8 (-15)	Hampson (1980)	0.02	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	10.5	DuPont (1969)	
WATER SOLUBILITY (mol. m^{-3})	34.7	DuPont (1969)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.9 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Chemical Name: Fluorocarbon-113

Chemical NO.: 56

Chemical Formula: CCl_2FCClF_2 (M.W.=187.5)

CAS Registry NO.: 75-13-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.015	0.50		0.0		400	0.0		Lillian et al (1975)
1.0	0.11	2.7	0.06		7	3.0		Wilson and Doyle (1970)
1.0	0.20	1.1	0.06		7	4.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	< 3.0 (-16)	Hampson (1980)	0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.4 (-1)	DuPont (1969)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	9.1 (-1)	DuPont (1969)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	4.9 (-1)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Unreactive in the troposphere. The loss rate measured by Wilson and Doyle (1970) is comparable to the inadvertant dilution rate in their smog chamber.

Chemical Name: Fluorocarbon-114 **Chemical NO.:** 57

Chemical Formula: $CClF_2CClF_2$ (M.W.=171) **CAS Registry NO.:** 75-14-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	< 1.0 (-16)	Hampson (1980)	≈ 0.0	
O_3	$cm^3 molec^{-1} s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.18	DuPont (1969)	
WATER SOLUBILITY (mol. m^{-3})	7.6 (-1)	DuPont (1969)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.3		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Unreactive in the troposphere.

Chemical Name: Formaldehyde **Chemical NO.:** 58

Chemical Formula: HCHO (M.W.=30) **CAS Registry NO.:** 50-00-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.2	0.5	0.44	0.59		10-12			Jefferies et al (1982)
1.0	0.5	0.14	0.14		6		8.0	Dimitriades and Wesson (1972)
3.6	0.2		0.43		3			Altshuller et al (1966)
5.6	0.05		0.44		3			Altshuller et al (1966)
6.1	0.9		1.05		3			Altshuller et al (1966)
5.0	3.0	0.0			3.3		20.0	Altshuller and Cohen (1963)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.1 (-11)	Stief et al (1980)	35.4	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}	5.0 (-5)	Calvert (1980)		

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.56	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	18.3	Merck (1976)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	5.5 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

An intermediate product of hydrocarbon oxidation in virtually all photochemical systems (Altshuller and Bufalini, 1971; Calvert, 1980). Typical products are CO, H_2 and H_2O_2.

Chemical Name: Glycerine **Chemical NO.:** 59

Chemical Formula: $HOCH_2CHOHCH_2OH$ (M.W.=91) **CAS Registry NO.:** 56-81-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.6 (-12)	Estimated	5.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.5 (-7)	Cammenga et al (1977)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	$20^\circ C$
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.5 (-11)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** II **OVERALL:** II

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are avilable.

Chemical Name: Hexamethylenetetramine (Formin)

Chemical NO.: 60

Chemical Formula: $C_6H_{12}N_4$ (M.W.=140)

CAS Registry NO.: 100-97-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_3 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.0 (-10)	Estimated	322.5	Rate extremely fast. Approaching the collision frequency.
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.7 (-7)		Estimated
WATER SOLUBILITY (mol. m^{-3})	4755	Merck (1976)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	1.6 (-10)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	570 22	Merck (1976)	alcohol ether
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** II **OVERALL:** II

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Heptenes

Chemical NO.: 61

Chemical Formula: C_7H_{14} (M.W.=98)

CAS Registry NO.: 592-76-7 (1-Heptene)

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
5.0	1.5	0.05	0.68	1.5	6	40		Miller and Joseph (1976)
3.0	1.0	>20	0.72	1.0	3	43		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.5 (-11)	Atkinson et al (1979)	113.0	rate constants for 1-Heptene
O_3	$cm^3\ molec^{-1}\ s^{-1}$	8.5 (-18)	NAS (1976)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.0 (-2)to7.4(-2	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	1.9 (-1)	Tewari et al (1982)	1-heptene
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.9 (-1)		1-heptene, calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Other Heptenes (such as 2-Heptene, 3-Heptene) are roughly twice as reactive as 1-Heptene. Based on OH and O_3 reactivity depletion rates larger than 25%/h are possible for all Heptenes.

Chemical Name: 1,6-Hexanediamine

Chemical NO.: 62

Chemical Formula: $NH_2C_6H_{12}NH_2$ (M.W.=116)

CAS Registry NO.: 124-09-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.1 (-11)	Estimated	100.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.7 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	> 860	Merck (1976)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	<1.9 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	slightly soluble	Merck (1976)	alcohol, benzene
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Hydrogen Cyanide

Chemical NO.: 63

Chemical Formula: HCN (M.W.=27)

CAS Registry NO.: 74-90-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	<1.0 (-15)	Phillips (1978)	≈ 0.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.7 (-1)	Dreisbach (1961)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	5.7 (-5)		calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available. The molecule appears to be virtually unreactive in the troposphere.

Chemical Name: Isodecyl alcohol

Chemical NO.: 64

Chemical Formula: $(CH_3)_2CH(CH_2)_6CH_2OH$ (M.W.=158)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	1.0 (-11)	Estimated	32.2	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.0 (-7)		Estimate
WATER SOLUBILITY (mol. m^{-3})	insoluble	Merck (1976)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

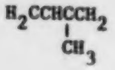
VOLATILITY: II

OVERALL: II

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Isoprene

Chemical Formula: 
$H_2CCHCCH_2$ with CH_3 below (M.W.=68)

Chemical NO.: 65

CAS Registry NO.: 78-79-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.8	0.2	0.3	0.66		10-12			Jefferies et al (1982)
0.2-13	0.33	0.0	0.06to 0.6		6	50-100		Arnts et al (1981)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	9.3 (-11)	Kleindienst et al (1982)	300.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.5 (-17)	Arnts et al (1981)		
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.5 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	9.2		Estimated
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	8.1 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Highly reactive and can produce significant ozone. Optimum OC/NO_x ratio is about 2. Identified products are formaldehyde, carbon monoxide, formic acid, methacrolein, methyl vinyl ketone, carbon dioxide, peroxyacetyl nitrate and nitric acid.

Chemical Name: Isopropyl alcohol

Chemical NO.: 66

Chemical Formula: $(CH_3)_2CHOH$ (M.W.=60)

CAS Registry NO.: 67-63-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.32	8.6		3.3		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.01		5	4.0	3.2	Yanagihara et al (1977)
1.0	0.6	0.05	1xtoluene		5	6.8	0.5xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.09		6		6.3	Levy and Miller (1970)
1.0	0.13	0.17	0.11		7	5.0		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.5 (-12)	Atkinson et al (1979)	17.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.8 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20°C
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.5 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Chemical Name: n-Propyl alcohol

Chemical NO.: 67

Chemical Formula: C_3H_7OH (M.W.=60)

CAS Registry NO.: 71-23-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	5.3 (-12)	Atkinson et al (1979)	17.1	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.6 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.6 (-6)		calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

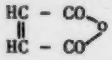
E. GENERAL COMMENTS

Considered reactive by analogy with isopropyl alcohol.

Chemical Name: Maleic anhydride

Chemical NO.: 68

Chemical Formula:



$$\begin{matrix} HC - CO \\ \| \\ HC - CO \end{matrix} \rangle O$$

CAS Registry NO.: 108-31-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.0 (-11)	Estimated	193.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.4(-4)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	reacts to maleic acid
HENRY'S CONSTANT (atm. m^3 mol^{-1})	8.2 (-9)		calculated
SOLVENT SOLUBILITY (mol. m^{-3})	5100 5400 2400	Merck (1976)	benzene chloroform toluene
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Methanol

Chemical NO.: 69

Chemical Formula: CH_3OH (M.W.=32)

CAS Registry NO.: 67-56-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.11	0.20	10.8				Joshi et al (1982)
4.0	0.2	0.25	0.33		10-12		1.8xpropane	Sickles et al (1980)
4.0	0.07	0.75	0.75		10-12		1.3xpropane	Sickles et al (1980)
4.0	0.2		0.25	12.3		1.3		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	0.0	1.4	Yanagihara et al (1977)
5.0	3.0	0.0					5-10	Altshuller and Cohen (1963)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.1 (-12)	Atkinson et al. (1979)	3.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.6 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.5 (-6)	Atkinson et al (1979)	calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	ethanol, ether, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Chemical Name: Methyl chloride

Chemical NO.: 70

Chemical Formula: CH_3Cl (M.W.=50.5)

CAS Registry NO.: 74-87-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.4 (-14)	Hampson (1980)	0.14	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.7	Dreisbach (1959	
WATER SOLUBILITY (mol. m^{-3})	107	Dilling (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.4 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Significantly less reactive than ethane.

Chemical Name: Methylene chloride **Chemical NO.:** 71

Chemical Formula: CH_2Cl_2 (M.W.=85) **CAS Registry NO.:** 75-09-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.07	0.25	0.1		10-12		0.6xpropane	Sickles et al (1980)
4.0	0.2		0.03	1.8		5.7		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	1.9	1.4	Yanagihara et al (1977)
1.0	0.1	2.0	0.06		7	5.5		Wilson and Doyle (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.6 (-13)	Hampson (1980)	0.5	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.7 (-1)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	200	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.9 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

The reactivity of Methylene chloride is less than ethane. Dilling et al (1976) show loss of 5% in 21 h irradiation. The high loss rate in the results of Wilson and Doyle (1970) is explicable as an uncontrolled dilution rate. However, the data of Dimitriades and Joshi (1977) cannot be explained. Sickles et al (1980) O_3 levels are indistinguishable from background.

Chemical Name: Methyl ethyl ketone **Chemical NO.:** 72

Chemical Formula: $CH_3COC_2H_5$ (M.W.=72) **CAS Registry NO.:** 78-93-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.5	0.18	0.38	0.55		10-12			Jefferies et al (1982)
4.0	0.2		0.3	8.3		1.5		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.01		5	2.2	2.1	Yanagihara et al (1977)
1.0	0.6	0.05	0.9xtoluene		5	2.4	0.6xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.28		6		9.4	Levy and Miller (1970)
1.0	0.15	3.7	0.12		7	5.5		Wilson and Doyle (1970)
4.0	1.0	0.1	0.32	4.0	6	11.4		Brunelle et al (1966)
8.0	2.0	0.1	0.23	6.0	6	9.4		Brunelle et al (1966)
3.0	1.0	>20	0.0		3			Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.4 (-12)	Atkinson et al (1979)	10.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	3600	Morrison and Boyd (1973)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.5 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Highly effective in NO→NO_2 conversion (Cox et al, 1980).

Chemical Name: Methyl isobutyl ketone **Chemical NO.:** 73

Chemical Formula: $(CH_3)_3CCOCH_3$ (M.W.=100) **CAS Registry NO.:** 108-10-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.26		5	5.0	7.2	Yanagihara et al (1977)
1.0	0.6	0.05	1.4xtoluene		5	4.8	1.7xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.45		6		17.2	Levy and Miller (1970)
1.0	0.2	2.4	0.15		7	8.0		Wilson and Doyle (1970)
8.0	2.0	0.02	0.5		6	8.3		Brunelle et al (1966)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.4 (-11)	Atkinson et al (1979)	45.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.9 (-2)	Weast (1973)	
WATER SOLUBILITY (mol. m^{-3})	190	Morrison and Boyd (1973)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.0 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, benzene, ether
PHYSICAL STATE	liquid		

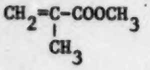
D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Methyl methacrylate

Chemical NO.: 74

Chemical Formula: 

$CH_2=C(CH_3)-COOCH_3$ (M.W.=100)

CAS Registry NO.: 80-62-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	2.0	0.11	0.73	4.4				Joshi et al (1982)
4.0	0.2	0.11	0.20	1.4				Joshi et al (1982)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.0 (-11)	Estimated	161.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.1 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	18.9		Estimated
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.7 (-3)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III   **VOLATILITY:** III   **OVERALL:** III

E. GENERAL COMMENTS

Chemical Name: Solvent naphtha **Chemical NO.:** 75

Chemical Formula: Mixture of C_5-C_{20} aliphatics **CAS Registry NO.:** 8030-30-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0^*	2.0	0.0	0.58	9.0	16.5	8.6		Brunelle et al (1966)
4.0^{**}	2.0	0.0	0.58	7.0	16.5	7.9		Brunelle et al (1966)
$4.0^{\dagger}$	2.0	0.0	0.53	9.0	16.5	4.8		Brunelle et al (1966)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	$\approx 10^{-11}$	Estimated	≈ 32	Reactivity assumed to be in the C_8-C_{10} alkane range
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.6 (-2)		Estimated
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Reactive aliphatic solvent mixture

*VM and P Naptha; **Mineral Spirits; †Eastern Stoddard solvent

Chemical Name: Naphthalene

Chemical NO.: 76

Chemical Formula: $C_{10}H_8$ (M.W.=128)

CAS Registry NO.: 91-20-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.4	0.97		0.0		4			Spicer et al (1974)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.6 (-11)	Estimated	51.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.8 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	3.1 (-1)	Dreisbach (1955)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	4.3 (-4)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	5400 5130 940	Dreisbach (1955)	acetone benzene ethanol
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: II

VOLATILITY: III

OVERALL: II

E. GENERAL COMMENTS

A free radical scavenger. Although highly reactive, it is unable to form significant ozone. High OC/NO_x irradiations have not been performed. Leads to significant aerosol formation (Spicer et al, 1974).

Chemical Name: Nitrobenzene **Chemical NO.:** 77

Chemical Formula: $C_6H_5NO_2$ (M.W.=123) **CAS Registry NO.:** 98-95-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.01		10-12			Sickles et al (1980)
4.0	0.067	0.25	0.02		10-12			Sickles et al (1980)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	2.1 (-13)	Zetzsch (1983)	0.7	
O_3	$cm^3 molec^{-1} s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.7 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	16	Merck (1976)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.3 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

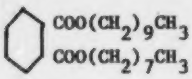
E. GENERAL COMMENTS

Also a smog inhibitor (Gitchell et al, 1974a).

Chemical Name: n-Octyl-n-decyl phthalate

Chemical NO.: 78

Chemical Formula:



(M.W.=418)

CAS Registry NO.: 1323-73-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.7 (-11)	Estimated	54.8	Not strictly amenable to estimate
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.1 (-9)		Estimated from boiling point data
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE			

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** I **OVERALL:** I

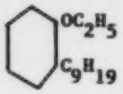
E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Nonyl phenol (ethoxylated)

Chemical NO.: 79

Chemical Formula:



(M.W.=248)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.7 (-11)	Estimated	151.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)			No estimates possible
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE			

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** II **OVERALL:** II

E. GENERAL COMMENTS

Chemical Name: Perchloroethylene **Chemical NO.:** 80

Chemical Formula: C_2Cl_4 (M.W.=166) **CAS Registry NO.:** 127-18-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.54		10–12		1.2xpropane	Sickles et al (1980)
4.0	0.07	0.25	1.19		10–12		1.6xpropane	Sickles et al (1980)
4.0	0.2		0.49	1.8		12.8		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.0		5	0.2	1.9	Yanagihara et al (1977)
5.0	1.77		0.07	4.5		2.0		Gay et al (1976)
0.85	0.48		0.5	7.0	9	12.5		Lillian et al (1975)
6.4	2.0	0.02	0.0		7	6.0		Brunelle et al (1966)
3.0	1.0		0.05		6			Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	1.7 (-13)	Hampson (1980)	0.5	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.4 (-2)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	9.0 (-1)	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3 mol^{-1}$)	2.7 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II **VOLATILITY:** III **OVERALL:** II

E. GENERAL COMMENTS

Because of Cl atom initiated oxidation of C_2Cl_4; somg chambers do not simulate the atmosphere. In the absence of Cl radicals, OH reactivity is dominant but too slow. These findings have recently been reviewed by Dimitriades et al (1983). Smog chamber reaction products are trichloroacetyl chloride, phosgene, hydrochloric acid, carbon monoxide, and formic acid.

Chemical Name: Phenol

Chemical NO.: 81

Chemical Formula: C_6H_5OH (M.W.=94)

CAS Registry NO.: 108-95-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	0.25	0.03		10-12			Sickles et al (1980)
4.0	0.07	0.25	0.05		10-12		0.3xpropane	Sickles et al (1980)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	2.8 (-11)	Gusten et al (1981)	90.3	
NO_3	$cm^3 molec^{-1} s^{-1}$	2.0 (-12)	Carter et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.0 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	870	Dreisbach (1955)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	8.0 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	very soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: II

VOLATILITY: III

OVERALL: II

E. GENERAL COMMENTS

Although highly reactive, no evidence of O_3 formation is seen. Phenol is a known smog inhibitor and provides an efficient sink for NO_x (Gitchell et al, 1974). At night rapid removal could occur by reaction with NO_3 radicals (Carter et al, 1981).

Chemical Name: Phosgene **Chemical NO.:** 82

Chemical Formula: $COCl_2$ (M.W.-99) **CAS Registry NO.:** 75-44-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	<1.0 (-14)	Estimated	<0.03	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.9	Dreisbach (1961)	
WATER SOLUBILITY (mol. m^{-3})	decomposes	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

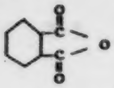
REACTIVITY: I **VOLATILITY:** III **OVERALL:** I

E. GENERAL COMMENTS

Formed as a by-product of chloroethylene oxidation (Gay et al, 1976). Shows no perceptible reactivity in smog chambers over a 24 h period (Singh, 1976). Most likely removal process is slow liquid phase hydrolysis. No laboratory kinetic or smog chamber data are available.

Chemical Name: Phthalic anhydride **Chemical NO.:** 83

Chemical Formula:



(M.W.=148) **CAS Registry NO.:** 85-44-9

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-11)	Estimated	38.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.8 (-7)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	42	Freier (1975)	Hydrolyzes to acid
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.6 (-8)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** II **OVERALL:** II

E. GENERAL COMMENTS

No laboratory or smog chamber data are available.

Chemical Name: Propane

Chemical NO.: 84

Chemical Formula: C_3H_8 (M.W.=44)

CAS Registry NO.: 74-98-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2	11	0.17	9.8				Joshi et al (1982)
4.0	2.0 to 0.0	0.25	0–0.48		10–12			Sickles et al (1980)*
4.0	0.2		0.08	3.6		2.0		Dimitriades and Joshi (1977)
2.0	1.0	0.05	0.03	5.0	5	4.1	3.3	Yanagihara et al (1977)
7.8	0.2	0.0	0.15		10	0.9		Zfonte and Bonamassa (1977)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.9 (-12)	Atkinson et al (1979)	6.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.3	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	1.4	McAuliffe (1966)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	7.1 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	6400	Hayduk (1972)	hexane
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Like other alkanes, propane/NO_x ratio is critical towards efficient oxidant formation. OC/NO_x ratio of 40-80 appears to be optimal. The stoichiometry for $NO \rightarrow NO_2$ conversion is comparable to that of propene after OH attack (Cox et al, 1980; Singh et al, 1981).

Chemical Name: Propylene

Chemical Formula: C_3H_6 (M.W.=42)

Chemical NO.: 85

CAS Registry NO.: 115-07-1

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
1.0	0.4	0.43	0.38		10-12			Jefferies et al (1982)
1.2	0.5	0.25	0.70		10-12	20.0		Kamens et al (1981)
2.0	1.0	0.05	0.49	3.8	5	19.0	14.0	Yanagihara et al (1977)
0.53	0.59		0.3		7	15.0	3.0	Finlayson and Pitts (1976)
1.0	0.5	0.11	0.71		6		8.8	Dimitriades et al (1975)
1.0	0.6	0.05	1.9x toluene		5	27.2	2xtoluene	Laity et al (1973)
1.0	0.5	0.11	0.68				10.1	Dimitriades and Wesson (1972)
2.0	1.0	0.05	0.54		6	12.1	12.1	Heuss and Glasson (1968)
3.0	1.0	>20	0.68	1.3	3	43.0		Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.5 (-11)	Atkinson et al (1979)	80.6	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.0 (-17)	Niki (1979)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	11.4	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	4.8	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	2.1 (-1)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

One of the most extensively studied and modeled OC/NO_x system (Altshuller and Bufalini, 1971; Finlayson and Pitts, 1976; Niki, 1979; Akimoto et al, 1979). Products include formaldehyde, acetaldehyde, formic acid, PAN, nitric acid, propylene oxide, propionaldehyde, methyl, ethyl and i-propyl nitrates; propeneglycol dinitrate and diacetyl acetone.

Chemical Name: Propylene glycol

Chemical NO.: 86

Chemical Formula: $CH_3CHOHCH_2OH$ (M.W.=76)

CAS Registry NO.: 57-55-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.4 (-12)	Estimated	20.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.8 (-4)	Jordan (1954)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	inf.	Freier (1975)	20°C
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	1.7 (-8)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	acetone, chloroform
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

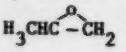
REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Propylene oxide

Chemical NO.: 87

Chemical Formula: 
$H_3CHC\overset{O}{\frown}CH_2$ (M.W.=58)

CAS Registry NO.: 75-56-9

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.3 (-12)	Atkinson et al (1979)	4.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.7 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	9100	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	7.4 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: II

VOLATILITY: III

OVERALL: II

E. GENERAL COMMENTS

Chemical Name: Styrene

Chemical NO.: 88

Chemical Formula: $C_6H_5CH{=}CH_2$ (M.W.=104)

CAS Registry NO.: 100-42-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.18	5.0	5	18.0	6.1	Yanagihara et al (1977)
4.0	2.0	0.0	0.31	5.6	6		10.5	Levy and Miller (1970)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.2 (-11)	Estimated	103.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	3.0 (-17)	NAS (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.0 (-3)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	1.5	Banerjee et al (1980)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	5.2 (-3)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

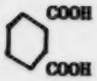
E. GENERAL COMMENTS

Reacts to form products with high-eye irritation index. Major product likely to be PBzN.

Chemical Name: Terephthalic acid

Chemical NO.: 89

Chemical Formula:



(M.W.=166)

CAS Registry NO.: 100-21-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	8.0 (-12)	Estimated	25.8	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.8 (-6)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	9.6 (-2)	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	9.1 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

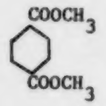
E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Terephthalic acid (dimethyl ester)

Chemical NO.: 90

Chemical Formula:



(M.W.=194)

CAS Registry NO.: 120-61-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$				
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)			
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE			

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

This is just another name of chemical No. 37 (Dimethyl terephthalate). It is, therefore, omitted from our list of chemicals.

Chemical Name: Tetrapropylene

Chemical NO.: 91

Chemical Formula: $C_{12}H_{24}$ (M.W.=168)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.7 (-11)	Estimated	19.4	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	4.6 (-4)		Estimated from boiling point data
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Toluene

Chemical NO.: 92

Chemical Formula: $C_6H_5CH_3$ (M.W.=92)

CAS Registry NO.: 108-88-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
2.2	0.34	0.25	0.40		10-12			Jefferies et al (1982)
1.1	0.49		0.3	6.0	6	8.3	2.4	Hendry (1979)
2.0	1.0	0.05	0.25	5.0	5	8.0	5.0	Yanagihara et al (1977)
1.0	0.5	0.11	0.36		6		4.4	Dimitriades et al (1975)
4.0	2.0	0.0	0.44	3.3	6		10.4	Levy and Miller (1970)
1.0	0.16	0.6	0.10		7	6.0		Wilson and Doyle (1970)
8.0	2.0	0.05	0.27	4.0	6			Brunelle et al (1966)
5.0	3.0	0.0	0.56	3.0	3		15.0	Altshuller and Cohen (1963)
1.9	0.1	0.0	0.36	3.0	3	12.3		Altshuller and Cohen (1963)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	5.8 (-12)	Atkinson et al (1979)	18.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.5 (-22)	NAS (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.7 (-2)	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	5.6	McAuliffe (1966)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	6.7 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, acetone, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

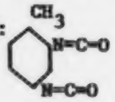
E. GENERAL COMMENTS

Kinetics of the photoxidation of toluene have been studied extensively (Hendry, 1979; O'Brien et al, 1979). A number of smog chamber runs summarized by O'Brien et al (1979) clearly show significant ozone and PAN formation for all toluene initial concentrations exceeding 1 ppm. Identified products are carbon monoxide, formaldehyde, acetaldehyde, peroxyacetyl nitrate, benzaldehyde, cresols, unsat. bi-functional aliphatic prouducts, dicarbonyls and nitrotoluenes.

Chemical Name: Toluene Diisocyanate

Chemical NO.: 93

Chemical Formula:



(M.W.=174)

CAS Registry NO.:

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.0 (-11)	Estimated	32.2	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.1 (-5)		Estimated (2,4 isomer)
WATER SOLUBILITY (mol. m^{-3})	reacts	Merck (1976)	2,4 - isomer
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	ether, acetone, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

This chemical may play a chain terminating role, typical of smog inhibitors.

Chemical Name: 1,1,1 Trichloroethane

Chemical NO.: 94

Chemical Formula: CH_3CCl_3 (M.W.=133.5)

CAS Registry NO.: 71-55-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	0.2		0.0	4.6		0.1		Dimitriades and Joshi (1977)
0.02	0.5		0.0		19	0.0		Lillian et al (1975)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-14)	Hampson (1980)	0.04	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.6 (-1)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	5.4	Dilling (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.0 (-2)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	acetone, benzene, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: I

VOLATILITY: III

OVERALL: I

E. GENERAL COMMENTS

Significantly less reactive than ethane.

Chemical Name: Trichloroethylene **Chemical NO.:** 95

Chemical Formula: C_2HCl_3 (M.W.=131.5) **CAS Registry NO.:** 79-01-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.11	5.0	5	9.4	5.4	Yanagihara et al (1977)
3.4	1.3	>20	0.24	1.8	3.3	29.0		Gay et al (1976)
1.0	0.7	>20	0.70	3.0	24	7.0	-70.0	Appleby (1976)
4.0	1.0	0.02	0.51	6.0	16.5	10.7		Brunelle et al (1966)
4.0	2.0	0.02	0.50	11.5	16.5	14.0		Brunelle et al (1966)
3.0	1.0	>20	0.0		6			Schuck and Doule (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.2 (-12)	Atkinson et al (1979)	7.1	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.8 (-2)	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	8.4	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	1.2 (-2)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	ether, alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Some Cl atom interactions may occur in smog chamber data. However, this chemical is sufficiently reactive with OH radicals to lead to ozone formation. Measured products in smog chambers are dichloroacetyl chloride, phosgene, hydrogenchloride, nitric acid, formic acid and carbon monoxide.

Chemical Name: Triethylene glycol **Chemical NO.:** 96

Chemical Formula: $(CH_2OHCH_2OCH_2)_2$ (M.W.=150) **CAS Registry NO.:** 112-27-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	2.7 (-11)	Estimated	87.0	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.7 (-6)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Freier (1975)	20°C
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	1.0 (-10)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Vinyl acetate monomer

Chemical NO.: 97

Chemical Formula: $CH_3COOCH{=}CH_2$ (M.W.=86)

CAS Registry NO.: 108-05-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.0	2.0	0.11	0.40	17.4				Joshi et al (1982)
4.0	0.2	0.11	0.34	3.6				Joshi et al (1982)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.0 (-11)	Estimated	96.8	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.5 (-1)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	290	Verschueren (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	5.2 (-4)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

Chemical Name: Vinyl chloride monomer **Chemical NO.:** 98

Chemical Formula: $CH_2{=}CHCl$ (M.W.=62.5) **CAS Registry NO.:** 75-01-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
4.6	1.5	>20	1.3*	3.0	3	14.0		Gay et al (1976)
1.7	1.0	0.0	0.45*	5.5	6	6.0		Gay et al (1976)
10.0	4.5	>20	2.0	5.0	9.5	9.0		Appleby (1976)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.6 (-12)	Atkinson et al(1979)	21.3	
O_3	$cm^3\ molec^{-1}\ s^{-1}$	1.9 (-19)	Gay et al (1976)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.5	Dreisbach (1959)	
WATER SOLUBILITY (mol. m^{-3})	1.8 (-2)	Verschueren (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	57		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	gas		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Known products are formaldehyde, formic acid, hydrogen chloride and CO.

*ozone still increasing

Chemical Name: m-and mixed Xylenes **Chemical NO.:** 99

Chemical Formula: 1,3-$C_6H_4(CH_3)_2$ (M.W.-106) **CAS Registry NO.:** 108-38-3 (m-xylene)
1330-20-7 (mixed)

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0*	1.0	0.05	0.49	2.8	5	11.9	10.2	Yanagihara et al (1977)
1.0	0.6	0.05	1.7x toluene		5	19.6	2xtoluene	Laity et al (1973)
4.0	2.0	0.0	0.45	1.1	6		26.7	Levy and Miller (1970)
2.0	1.0	0.0	0.39	6.0	6	9.0	15.5	Heuss and Glasson (1968)
4.0	2.0	0.02	0.54	3.5	6	10.8		Brunelle et al (1966)
5.0	3.0	0.0	1.0		2.2		70.0	Altshuller and Cohen (1963)
6.0	1.0	> 20	0.18	0.9	3			Schuck and Doyle (1959)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	2.1 (-11)	Atkinson et al (1979)	67.7	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.1 (-2)	Zwolinski and Wilhoit(1971)	m-Xylene only
WATER SOLUBILITY (mol. m^{-3})	1.5	Polak and Lu (1973)	m-Xylene only
HENRY'S CONSTANT (atm. m^3 mol^{-1})	7.0 (-3)	Mackay and Shiu (1981)	m-Xylene only
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Product of m-Xylene photooxidation are peroxyacetyl nitrate, carbon monoxide, formaldehyde, methyl glyoxal, nitric acid, aliphatic dicarbonyls,acetaldehyde, and m-tolualdehyde

*mixed Xylenes

Chemical Name: o-Xylene **Chemical NO.:** 100

Chemical Formula: 1,2-$C_6H_4(CH_3)_2$ (M.W.=106) **CAS Registry NO.:** 95-47-6

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
0.6	0.32	0.33	0.51		10-12			Jefferies et al (1982)
2.0	1.0	0.05	0.51	2.5	5	11.1	13.1	Yanagihara et al (1977)
1.0	0.5	0.11	0.53		6	5.4		Dimitriades et al (1975)
1.0	0.6	0.05	1.8x toluene		5	12.8	1.5xtoluene	Laity et al (1973)
2.0	1.0	0.05	0.32	6.0	6	8.7	13.6	Heuss and Glasson (1968)
4.0	1.0	0.02	0.32	2.0	6			Brunelle et al (1966)
5.0	3.0	0.0	0.7		2		40.0	Altshuller and Cohen (1963)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-11)	Atkinson et al (1979)	38.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	8.7 (-3)	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	2.0	Polak and Lu (1973)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	4.4 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Xylenes are about half as efficient in ozone formation as propene (Cox et al, 1980). Known photodegradation products are formaldehyde, peroxyacetyl nitrate, biacetyl, glyoxal methyl, glyoxal o-tolualdehyde, 3,4-dimethyl nitro-benzene, 2,3-dimethyl-nitro benzene, and o-methylbenzyl nitrate.

Chemical Name: p-Xylene

Chemical NO.: 101

Chemical Formula: $1,4\text{-}C_6H_4(CH_3)_2$ (M.W.-106)

CAS Registry NO.: 106-42-3

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				
2.0	1.0	0.05	0.39	4.5	5	10.7	7.8	Yanagihara et al (1977)
1.0	0.5	0.11	0.49		6		5.4	Dimitriades et al (1975)
2.0	1.0	0.05	0.26	6.0	6	7.0	7.7	Heuss and Glasson (1968)
5.0	3.0	0.0	0.65	2.5			30.0	Altshuller and Cohen (1963)

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.1 (-11)	Atkinson et al (1979)	35.4	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.2 (-2)	Zwolinski and Wilhoit(1971)	
WATER SOLUBILITY (mol. m^{-3})	1.7	Polak and Lu (1973)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	6.7 (-3)	Mackay and Shiu (1981)	
SOLVENT SOLUBILITY (mol. m^{-3})	soluble	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Products similar to o- and m-Xylenes.

Chemical Name: Dimethyl succinate

Chemical NO.: 102

Chemical Formula: $CH_3OOC(CH_2)_2COOCH_3$ (M.W.=146)

CAS Registry NO.: 106-65-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	3.0 (-12)	Estimated	10.0	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	6.4 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	57	Merck (1976)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	1.1 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	200	Merck (1976)	alcohol
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Dimethyl glutarate

Chemical NO.: 103

Chemical Formula: $CH_3OOC(CH_2)_3COOCH_3$ (M.W.=160)

CAS Registry NO.: 1119-40-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.0 (-12)	Estimated	12.9	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	3.2 (-4)		Estimated
WATER SOLUBILITY (mol. m^{-3})	7.8		Estimated
HENRY'S CONSTANT (atm. m^3 mol^{-1})	4.1 (-5)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Dimethyl adipate

Chemical NO.: 104

Chemical Formula: $CH_3OOC(CH_2)_4COOCH_3$ (M.W.=174)

CAS Registry NO.: 627-93-0

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.8 (-12)	Estimated	15.4	Not strictly amenable to estimation
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	9.9 (-5)		Estimated
WATER SOLUBILITY ($mol.\ m^{-3}$)	1.8		Estimated
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	5.5 (-5)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	liquid		
PHYSICAL STATE			

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: 2-Methoxy ethanol

Chemical NO.: 105

Chemical Formula: $CH_3OCH_2CH_2OH$ (M.W.=76)

CAS Registry NO.: 109-86-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	7.1 (-12)	Estimated	22.9	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.9 (-2)		Estimated
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Ethylene glycol monomethyl ether

Chemical NO.: 106

Chemical Formula: $HOCH_2CH_2OCH_3$ (M.W.=76)

CAS Registry NO.: 109-86-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	8.1 (-12)	Estimated	26.1	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.6 (-2)	Jordan (1954)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Mellan (1977)	20°C
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.3 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Ethylene glycol monoethyl ether **Chemical NO.:** 107

Chemical Formula: $HOCH_2CH_2OC_2H_5$ (M.W.=90) **CAS Registry NO.:** 110-80-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.4 (-11)	Estimated	45.2	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	7.0 (-3)	Mellan (1977)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	inf.	Mellan (1977)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	4.2 (-7)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Mellan (1977)	acetone, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

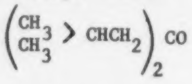
REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Diisoamyl ketone **Chemical NO.:** 108

Chemical Formula:



$\left(\begin{matrix}CH_3\\CH_3\end{matrix} > CHCH_2\right)_2 CO$ (M.W.=142) **CAS Registry NO.:**

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	8.0 (-12)	Estimated	25.8	
O_3	$cm^3 molec^{-1} s^{-1}$				
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)			No estimation is possible
WATER SOLUBILITY (mol. m^{-3})			
HENRY'S CONSTANT (atm. m^3 mol^{-1})			
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** II **OVERALL:** II

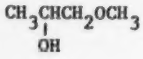
E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available. No vapor pressure estimation was possible.

Chemical Name: Propylene glycol methyl ether

Chemical NO.: 109

Chemical Formula:



$CH_3CH(OH)CH_2OCH_3$ (M.W.=90)

CAS Registry NO.: 107-98-2

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_X	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	1.3 (-11)	Estimated	41.9	
O_3	$cm^3 molec^{-1} s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	1.4 (-2)	Mellan (1977)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Mellan (1977)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	8.6 (-7)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Mellan (1977)	acetone, benzene
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III

VOLATILITY: III

OVERALL: III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: Dipropylene glycol methyl ether **Chemical NO.:** 110

Chemical Formula: $CH_3(CHOH)_2CH_2CHOHCH_2OCH_3$ (M.W.=164) **CAS Registry NO.:** 34590-94-8

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-11)	Estimated	38.7	
O_3	$cm^3\ molec^{-1}\ s^{-1}$				
hν	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.3 (-4)	Mellan (1977)	
WATER SOLUBILITY (mol. m^{-3})	inf.	Mellan (1977)	
HENRY'S CONSTANT (atm. $m^3\ mol^{-1}$)	3.2 (-8)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

No smog chamber or laboratory kinetic data are available.

Chemical Name: o-cresol

Chemical NO.: 111A

Chemical Formula: $CH_3C_6H_4OH$ (M.W.=108)

CAS Registry NO.: 95-48-7

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	4.7 (-11)	Atkinson et al (1979)	151.6	
NO_3	$cm^3\ molec^{-1}\ s^{-1}$	1.2 (-11)	Carter et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	5.6 (-4)	Dreisbach (1955)	
WATER SOLUBILITY ($mol.\ m^{-3}$)	242	Freier (1975)	
HENRY'S CONSTANT ($atm.\ m^3\ mol^{-1}$)	2.3 (-6)		Calculated
SOLVENT SOLUBILITY ($mol.\ m^{-3}$)	inf.	Merck (1976)	alcohol, ether, chloroform
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

The major product of OH attack should be dihydroxytoluenes. In the presence of NO_x hydroxynitrotoluenes have been observed (Hendry, 1979). During nighttime effective removal via NO_3 radical attack could occur (Carter et al., 1981). Cresols (especially o and p), because of their aromatic ring and quinoidal resonance possibilities, may act as chain terminators. However, available evidence suggests that even chain terminators can produce ozone (Pitts et al., 1977; Cupitt and Corse, 1979).

Chemical Name: m-cresol

Chemical NO.: 111B

Chemical Formula: $CH_3C_6H_4OH$ (M.W.=108)

CAS Registry NO.: 108-39-4

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3\ molec^{-1}\ s^{-1}$	6.7 (-11)	Atkinson et al (1979)	216.1	
NO_3	$cm^3\ molec^{-1}\ s^{-1}$	7.0 (-12)	Carter et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.5 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	26	Tewari et al (1982)	
HENRY'S CONSTANT (atm. m^3 mol^{-1})	9.6 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})	inf.	Merck (1976)	alcohol, ether, chloroform
PHYSICAL STATE	liquid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Same as o-cresol.

Chemical Name: p-cresol

Chemical NO.: 111C

Chemical Formula: $CH_3C_6H_4OH$ (M.W.=108)

CAS Registry NO.: 106-44-5

A. SMOG CHAMBER DATA

INITIAL CONC. (PPM)			MAX. O_3		TOTAL IRRADIATION TIME (h)	AVERAGE OC DISAPPEARANCE RATE (%/h)	NO_2 FORMATION RATE (PPB/Min)	REFERENCES
ORGANIC CHEMICAL (OC)	NO_x	NO_2/NO	CONC. (PPM)	TIME (h)				

B. KINETIC DATA

REACTION WITH	UNITS	RATE CONSTANT VALUE (25°C)	REFERENCES	OH RATE CONST. RELATIVE TO ETHANE	COMMENTS ON RATE CONSTANT ESTIMATION
OH	$cm^3 molec^{-1} s^{-1}$	5.2 (-11)	Atkinson et al(1979)	167.7	
No_3	$cm^3 molec^{-1} s^{-1}$	1.3 (-11)	Carter et al (1981)		
$h\nu$	s^{-1}				

C. VOLATILITY DATA

PROPERTY NAME (UNITS)	PROPERTY VALUE (25°C)	REFERENCES	COMMENTS
VAPOR PRESSURE (atm.)	2.6 (-4)	Dreisbach (1955)	
WATER SOLUBILITY (mol. m^{-3})	213	Morrison and Boyd (1973)	
HENRY'S CONSTANT (atm. $m^3 mol^{-1}$)	1.2 (-6)		Calculated
SOLVENT SOLUBILITY (mol. m^{-3})			
PHYSICAL STATE	solid		

D. CLASSIFICATIONS

REACTIVITY: III **VOLATILITY:** III **OVERALL:** III

E. GENERAL COMMENTS

Same as o-cresol.